Supporting Information

Ring Opening versus Ring Expansion in Rearrangement of Bicyclic Cyclobutylcarbinyl Radicals

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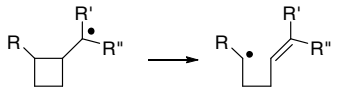
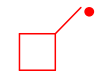
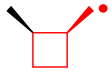
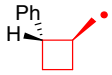
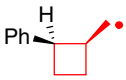
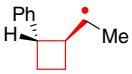
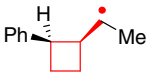
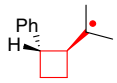
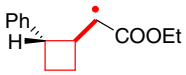
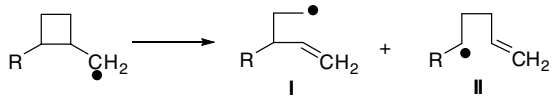
Table S1 Electronic energies (in a.u.) calculated at ONIOM(QCISD(T)/6-311+G(2df,2p):B3LYP/6-311+G(2df,2p)) and UB3LYP/ 6-311++G(2df,2p) level and thermal correction to Gibbs free energies (in a.u.) calculated at UB3LYP/6-31+G(d) for substituted cyclobutylcarbinyl radicals with known experimental ring-opening rates.

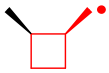
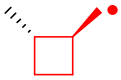
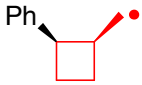
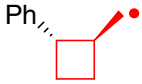
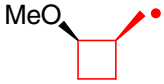
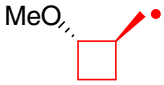
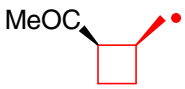
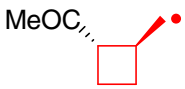


Compound Indices[a]		Electronic Energies by ONIOM method (a.u.)	Electronic Energies by B3LYP method(a.u.)	TCG (a.u.)
	**1a**	-195.458156	-195.926138	0.094595
	1a-TS	-195.434358	-195.906525	0.093929
	**1b**	-234.784749	-235.253086	0.121557
	1b-TS	-234.765432	-235.237860	0.120063
	**1c**	-426.582206	-427.049920	0.168157
	1c-TS	-426.570456	-427.041923	0.168556
	**1d**	-426.578269	-427.045625	0.168926
	1d-TS	-426.566268	-427.038354	0.168551
	**1e**	-465.915258	-466.383043	0.194875
	1e-TS	-465.902181	-466.373609	0.194270
	**1f**	-465.910930	-466.378671	0.195024
	1f-TS	-465.898305	-466.370458	0.193918
	**1g**	-505.245245	-505.713053	0.220528
	1g-TS	-505.231790	-505.703267	0.220208
	**1h**	-654.541445	-655.009231	0.205831
	1h-TS	-654.527049	-654.998794	0.205496

[a] The inner layer in the ONIOM method is highlighted in red.

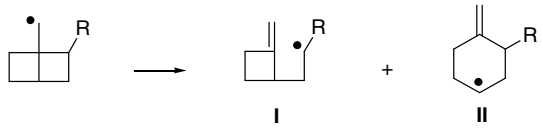
Table S2 Electronic energies (in a.u.) calculated at ONIOM(QCISD(T)/6-311+G(2df,2p):B3LYP/6-311+G(2df,2p)) level and thermal correction to Gibbs free energies (in a.u.) calculated at UB3LYP/6-31+G(d) for monocyclic cyclobutylcarbinyl radicals.



Compound Indices[a]		Electronic Energies (a.u.)	TCG (a.u.)
	**2a**	-195.458156	0.094595
	2a-TS	-195.434358	0.093929
	**2b**	-234.784749	0.121557
	2b-TSI	-234.760443	0.120616
	2b-TSII	-234.765432	0.120063
	**2c**	-234.788564	0.121017
	2c-TSI	-234.763826	0.11995
	2c-TSII	-234.767052	0.119998
	**2d**	-426.578269	0.168926
	2d-TSI	-426.551568	0.167608
	2d-TSII	-426.566268	0.168551
	**2e**	-426.582761	0.168701
	2e-TSI	-426.556346	0.166852
	2e-TSII	-426.570456	0.168556
	**2f**	-310.017661	0.123501
	2f-TSI	-309.992930	0.122811
	2f-TSII	-310.002975	0.123517
	**2g**	-310.021403	0.123648
	2g-TSI	-309.996393	0.122547
	2g-TSI	-310.005246	0.123360
	**2h**	-348.152566	0.127031
	2h-TSI	-348.125892	0.125783
	2h-TSII	-348.141529	0.126268
	**2i**	-348.156044	0.126450
	2i-TSI	-348.130170	0.124991
	2i-TSII	-348.144542	0.126597

[a] The inner layer is highlighted in red.

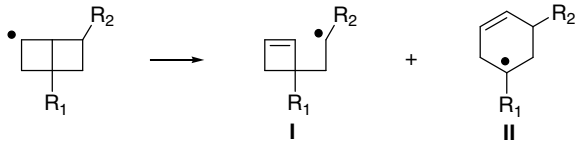
Table S3 Electronic energies (in a.u.) calculated at ONIOM(QCISD(T)/6-311+G(2df,2p):B3LYP/6-311+G(2df,2p)) level and thermal correction to Gibbs free energies (in a.u.) calculated at UB3LYP/6-31+G(d) for bicyclo[2.2.0]hexan-1-ylmethyl radicals.



Compound Indices[a]		Electronic Energies (a.u.)	TCG (a.u.)
(±) H	**3a**	-272.698219	0.126495
	3a-TSI	-272.670208	0.126091
	3a-TSII	-272.693573	0.126233
(±) Ph	**3b**	-503.988725	0.201208
	3b-TSI	-503.974789	0.200844
	3b-TSII	-503.982832	0.201124
(±) Ph	**3c**	-503.991168	0.201769
	3c-TSI	-503.974914	0.201060
	3c-TSII	-503.985444	0.201438
(±) COMe	**3d**	-425.564256	0.159409
	3d-TSI	-425.549521	0.158023
	3d-TSII	-425.558405	0.159196
(±) COMe	**3e**	-425.565561	0.159254
	3e-TSI	-425.550691	0.159184
	3e-TSII	-425.559787	0.158718

[a] The inner layer is highlighted in red.

Table S4 Electronic energies (in a.u.) calculated at ONIOM(QCISD(T)/6-311+G(2df,2p):B3LYP/6-311+G(2df,2p)) level and thermal correction to Gibbs free energies (in a.u.) calculated at UB3LYP/6-31+G(d) for bicyclo[2.2.0]hexan-2-yl radicals.

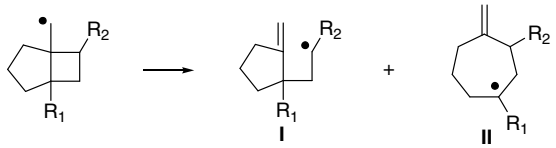


I II

Compound Indices [a]		Electronic Energies (a.u.)	TCG (a.u.)
(±) H	**4a**	-233.457057	0.101136
	4a-TSI	-233.430778	0.099379
	4a-TSII	-233.432020	0.100342
(±) Ph	**4b**	-464.582254	0.174296
	4b-TSI	-464.554657	0.172326
	4b-TSII	-464.565477	0.174877
(±) MeOC	**4c**	-386.154365	0.131664
	4c-TSI	-386.126514	0.130366
	4c-TSII	-386.141239	0.133479
(±) Ph	**4d**	-464.579866	0.174614
	4d-TSI	-464.566294	0.173902
	4d-TSII	-464.553762	0.174025
(±) Ph	**4e**	-464.579428	0.174689
	4e-TSI	-464.563190	0.174173
	4e-TSII	-464.552933	0.174125
(±) COMe	**4f**	-386.154663	0.132441
	4f-TSI	-386.141864	0.132066
	4f-TSII	-386.127260	0.131760
(±) COMe	**4g**	-386.153695	0.132087
	4g-TSI	-386.139504	0.131562
	4g-TSII	-386.127167	0.131397

[a] The inner layer is highlighted in red.

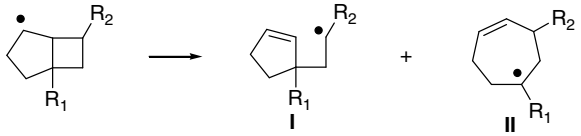
Table S5 Electronic energies (in a.u.) calculated at ONIOM(QCISD(T)/6-311+G(2df,2p):B3LYP/6-311+G(2df,2p)) level and thermal correction to Gibbs free energies (in a.u.) calculated at UB3LYP/6-31+G(d) for bicyclo[3.2.0]heptan-1-ylmethyl radicals.

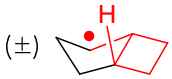
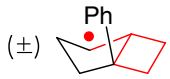
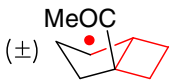


Compound Indices [a]		Electronic Energies (a.u.)	TCG (a.u.)
(±) H	**5a**	-312.226100	0.156566
	5a-TSI	-312.198146	0.154870
	5a-TSII	-312.209740	0.156278
(±) Ph	**5b**	-543.345501	0.231292
	5b-TSI	-543.316204	0.229321
	5b-TSII	-543.337499	0.230584
(±) MeOC	**5c**	-464.921118	0.189383
	5c-TSI	-464.891687	0.187532
	5c-TSII	-464.915748	0.189181
(±) Ph	**5d**	-543.345821	0.230322
	5d-TSI	-543.33195	0.229847
	5d-TSII	-543.327467	0.230185
(±) Ph	**5e**	-543.347463	0.230543
	5e-TSI	-543.333246	0.230064
	5e-TSII	-543.329791	0.230760
(±) COMe	**5f**	-464.921907	0.188824
	5f-TSI	-464.907358	0.187556
	5f-TSII	-464.904020	0.188212
(±) COMe	**5g**	-464.922654	0.189271
	5g-TSI	-464.90912	0.187993
	5g-TSII	-464.905166	0.188189

[a] The inner layer is highlighted in red.

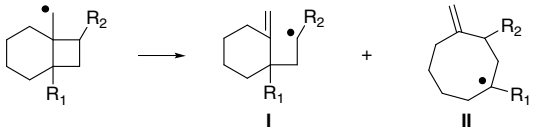
Table S6 Electronic energies (in a.u.) calculated at ONIOM(QCISD(T)/6-311+G(2df,2p):B3LYP/6-311+G(2df,2p)) level and thermal correction to Gibbs free energies (in a.u.) calculated at UB3LYP/6-31+G(d) for bicyclo[3.2.0]heptan-2-yl radicals.

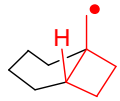
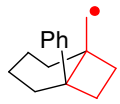
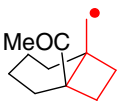
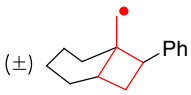
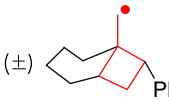
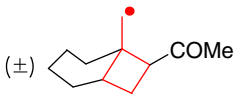
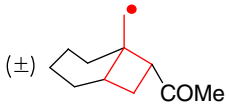


Compound Indices [a]		Electronic Energies (a.u.)	TCG (a.u.)
(±) 	**6a**	-272.903915	0.130469
	6a-TSI	-272.876341	0.128089
	6a-TSII	-272.870414	0.129166
(±) 	**6b**	-504.024912	0.204243
	6b-TSI	-503.997946	0.201897
	6b-TSII	-504.001299	0.203761
(±) 	**6c**	-425.598913	0.161827
	6c-TSI	-425.569712	0.158414
	6c-TSII	-425.579277	0.162831
(±) 	**6d**	-504.024048	0.203469
	6d-TSI	-504.011561	0.202405
	6d-TSII	-503.991793	0.203259
(±) 	**6e**	-504.026401	0.203228
	6e-TSI	-504.009880	0.203011
	6e-TSII	-503.988821	0.202881
(±) 	**6f**	-425.600969	0.161835
	6f-TSI	-425.587457	0.160545
	6f-TSII	-425.566670	0.160882
(±) 	**6g**	-425.600810	0.161629
	6g-TSI	-425.585897	0.160772
	6g-TSII	-425.560868	0.160232

[a] The inner layer is highlighted in red.

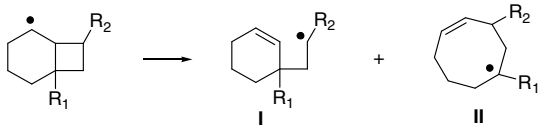
Table S7 Electronic energies (in a.u.) calculated at ONIOM(QCISD(T)/6-311+G(2df,2p):B3LYP/6-311+G(2df,2p)) level and thermal correction to Gibbs free energies (in a.u.) calculated at UB3LYP/6-31+G(d) for bicyclo[4.2.0]octan-1-ylmethanyl radicals.



Compound Indices [a]		Electronic Energies (a.u.)	TCG (a.u.)
(±) 	**7a**	-351.555490	0.184954
	7a-TSI	-351.531500	0.184135
	7a-TSII	-351.533489	0.184282
(±) 	**7b**	-582.667601	0.259958
	7b-TSI	-582.642156	0.259377
	7b-TSII	-582.657013	0.259148
(±) 	**7c**	-504.244253	0.218097
	7c-TSI	-504.218509	0.217144
	7c-TSII	-504.234986	0.218163
(±) 	**7d**	-582.674001	0.259153
	7d-TSI	-582.663346	0.258539
	7d-TSII	-582.649901	0.258583
(±) 	**7e**	-582.678306	0.258721
	7e-TSI	-582.667263	0.258892
	7e-TSII	-582.654789	0.258174
(±) 	**7f**	-504.249919	0.216793
	7f-TSI	-504.239167	0.216655
	7f-TSII	-504.225346	0.216176
(±) 	**7g**	-504.252447	0.216905
	7g-TSI	-504.242762	0.217117
	7g-TSII	-504.229205	0.216052

[a] The inner layer is highlighted in red.

Table S8 Electronic energies (in a.u.) calculated at ONIOM(QCISD(T)/6-311+G(2df,2p):B3LYP/6-311+G(2df,2p)) level and thermal correction to Gibbs free energies (in a.u.) calculated at UB3LYP/6-31+G(d) for bicyclo[4.2.0]octan-2-yl radicals.



Compound Indices[a]		Electronic Energies (a.u.)	TCG (a.u.)
(±) H	**8a**	-312.233408	0.158681
	8a-TSI	-312.209115	0.156812
	8a-TSII	-312.203528	0.157816
(±) Ph	**8b**	-543.355346	0.233030
	8b-TSI	-543.329439	0.230743
	8b-TSII	-543.334431	0.233290
(±) COMe	**8c**	-464.928019	0.190614
	8c-TSI	-464.901601	0.188553
	8c-TSII	-464.912335	0.191500
(±) Ph	**8d**	-543.357991	0.232494
	8d-TSI	-543.345237	0.231547
	8d-TSII	-543.325597	0.231280
(±) Ph	**8e**	-543.350731	0.232597
	8e-TSI	-543.338486	0.231408
	8e-TSII	-543.315340	0.232083
(±) COMe	**8f**	-464.931760	0.190091
	8f-TSI	-464.920613	0.189460
	8f-TSII	-464.899574	0.188670
(±) COMe	**8g**	-464.927238	0.190256
	8g-TSI	-464.916347	0.189154
	8g-TSII	-464.893327	0.190076

[a] The inner layer is highlighted in red.

The Cartesian coordinates (Å) of optimized structures by UB3LYP/6-31+G(d) method

*** The charge and spin of all molecules are 0 and 2.**

*** The number of imaginary frequencies of reactants is ZERO, and that of transition states is ONE.**

1a

C	-1.953013	-0.000083	0.152281
C	-0.584199	0.000064	-0.402045
C	0.451781	1.080548	0.082265
C	1.562025	-0.000060	0.035212
C	0.451628	-1.080517	0.081976
H	2.089336	0.000017	-0.925741
H	2.305484	-0.000189	0.839259
H	0.563985	1.974664	-0.541109
H	0.232924	1.393637	1.110033
H	-0.615376	0.000305	-1.498704
H	0.232725	-1.393801	1.109672
H	-2.836271	0.001377	-0.479571
H	-2.105927	-0.001202	1.229587
H	0.563795	-1.974523	-0.541555

1a-TS

C	0.809207	1.159157	-0.139372
C	1.532276	-0.167914	0.006915
C	0.289968	-1.071649	-0.094434
C	-0.751760	-0.083256	0.433261
C	-1.985489	0.132034	-0.150687
H	0.983364	1.974319	0.561382
H	0.545821	1.477547	-1.146476
H	1.993515	-0.249452	0.998579
H	2.314047	-0.360453	-0.740001
H	0.334960	-2.015778	0.465761
H	0.068393	-1.314017	-1.141477
H	-0.663530	0.143955	1.497378
H	-2.740441	0.748699	0.329903
H	-2.201337	-0.215052	-1.159144

1b

C	-1.985529	0.383346	-0.081338
C	-0.798615	-0.339887	0.416025
C	-0.069886	-1.363466	-0.514088
C	1.290873	-0.898317	0.063360
C	0.606483	0.399082	0.580833
H	1.634541	-1.541473	0.881546
H	2.118273	-0.767145	-0.644017
H	-0.347133	-2.416742	-0.395279
H	-0.184674	-1.093985	-1.570389
H	-1.030851	-0.820799	1.374591
H	-2.825500	0.618655	0.566241
H	-2.019457	0.765734	-1.098552
H	0.833442	0.667359	1.620296
C	0.819527	1.617102	-0.314466
H	0.167786	2.449175	-0.021610
H	1.859683	1.961312	-0.245797
H	0.616774	1.390750	-1.368979

1b-TS

C	-0.932969	-0.209170	0.578315
C	-0.936250	1.222370	0.052873
C	0.505606	1.232963	-0.490856
C	1.090283	0.134647	0.399939
C	1.889548	-0.895428	-0.066436
H	-1.149522	-0.360761	1.636986
H	-1.057025	1.941848	0.871613
H	-1.715919	1.432703	-0.692722
H	1.034140	2.193539	-0.421091
H	0.536263	0.915240	-1.540226
H	1.225941	0.423004	1.444083
H	2.399819	-1.570707	0.615608
H	1.947301	-1.132069	-1.126799
C	-1.391804	-1.319177	-0.323569
H	-1.053255	-2.297641	0.037710
H	-2.492893	-1.349466	-0.378314
H	-1.021334	-1.192923	-1.348448

1c

C	1.753135	-1.572494	0.169202
C	2.965919	-0.709690	-0.252387
C	2.003530	0.511717	-0.443428
C	0.989586	-0.264929	0.501464
H	1.314187	-2.084804	-0.693831
H	1.892639	-2.299758	0.974994
H	3.546630	-1.023316	-1.125356
H	3.652812	-0.536201	0.583388
H	1.597148	0.497658	-1.461507
H	1.218404	0.027920	1.535627
C	-0.490754	-0.124268	0.252060
C	-1.083269	1.149131	0.258434
C	-1.310916	-1.234922	0.017131
C	-2.449418	1.306219	0.032527
H	-0.460260	2.022715	0.437330
C	-2.681874	-1.081499	-0.204818
H	-0.878329	-2.231743	0.013552
C	-3.256186	0.189098	-0.200326
H	-2.886373	2.301738	0.038525
H	-3.299507	-1.958411	-0.382371
H	-4.321898	0.310054	-0.375807
C	2.454562	1.866947	-0.078107
H	2.328974	2.718507	-0.739001
H	2.929695	2.043786	0.883946

1c-TS

C	3.271130	0.076749	-0.328721
C	2.670833	1.093553	0.423528
C	1.323150	1.010602	0.765370
C	0.528423	-0.089975	0.369005
C	1.152299	-1.102703	-0.393446
C	2.502504	-1.020082	-0.733129
C	-0.892882	-0.109408	0.710315
C	-1.789030	-1.344914	0.713307
C	-2.981304	-0.659228	0.022264
C	-2.157080	0.402899	-0.713075
C	-2.525383	1.748559	-0.794269
H	-1.160450	0.610071	1.484767
H	-1.977688	-1.772329	1.706546
H	-1.382188	-2.141182	0.081417
H	-3.642118	-0.178285	0.754100
H	-3.599251	-1.291911	-0.627361

H	-1.579322	0.014738	-1.554955
H	-2.002683	2.439006	-1.450599
H	-3.256105	2.173721	-0.109254
H	0.866060	1.804776	1.352074
H	0.579105	-1.965644	-0.720748
H	3.257083	1.950400	0.746995
H	2.958271	-1.817296	-1.315691
H	4.323319	0.137614	-0.594185

1d

C	-1.778468	1.304982	1.317847
C	-2.069043	-0.071009	0.863511
C	-3.106507	-0.178523	-0.294878
C	-1.949960	-0.339455	-1.312933
C	-1.006805	-0.745824	-0.149347
H	-1.665980	0.621077	-1.755536
H	-2.072219	-1.067767	-2.122448
H	-1.083200	-1.828817	0.005686
H	-3.714269	-1.086230	-0.211982
H	-3.776495	0.678272	-0.425341
H	-2.254744	-0.717698	1.731295
H	-2.047909	2.169533	0.716227
H	-1.165689	1.482268	2.197019
C	0.447387	-0.360836	-0.126067
C	0.899834	0.893191	-0.569612
C	1.401232	-1.261902	0.375211
C	2.253582	1.233007	-0.512775
H	0.190522	1.614414	-0.965856
C	2.756559	-0.927438	0.436402
H	1.075942	-2.241712	0.720412
C	3.188880	0.324553	-0.008375
H	2.578186	2.209548	-0.864369
H	3.473149	-1.646101	0.826965
H	4.242553	0.588741	0.034020

1d-TS

C	0.967510	-0.007744	-1.009969
C	1.942387	-1.182329	-0.863578
C	2.637454	-0.670249	0.410918
C	2.250145	0.803514	0.242835

C	1.769497	1.596018	1.292387
H	1.061894	0.589264	-1.917278
H	2.632012	-1.211634	-1.715036
H	1.472029	-2.169838	-0.788378
H	3.718078	-0.850307	0.482344
H	2.170028	-1.077895	1.315296
H	2.839488	1.332928	-0.509360
H	1.668438	2.672863	1.185763
H	1.340334	1.147671	2.185329
C	-0.413193	-0.079785	-0.519228
C	-0.853934	-1.060278	0.394320
C	-1.349313	0.892240	-0.934234
C	-2.168257	-1.069936	0.863655
H	-0.166151	-1.827788	0.738108
C	-2.661265	0.884409	-0.465283
H	-1.034625	1.659762	-1.638688
C	-3.080188	-0.098922	0.438491
H	-2.482053	-1.840985	1.563452
H	-3.360730	1.643546	-0.807331
H	-4.103793	-0.109212	0.803893

1e

C	1.323094	-2.053604	0.310537
C	2.655688	-1.372910	-0.083449
C	1.887496	-0.039102	-0.309740
C	0.721780	-0.649864	0.603616
H	0.840558	-2.526994	-0.551053
H	1.332035	-2.770777	1.137608
H	3.212464	-1.780265	-0.933351
H	3.336914	-1.291200	0.771579
H	1.506031	0.002215	-1.339306
H	0.936756	-0.377882	1.643745
C	-0.713469	-0.327954	0.292271
C	-1.294647	-0.668953	-0.939833
C	-1.509159	0.348788	1.228522
C	-2.621351	-0.347433	-1.223308
H	-0.704034	-1.192752	-1.687841
C	-2.837524	0.673577	0.949741
H	-1.079526	0.620976	2.190360
C	-3.399821	0.325778	-0.278842
H	-3.049081	-0.623549	-2.183889
H	-3.432816	1.196389	1.694170

H	-4.434301	0.575490	-0.499201
C	2.507843	1.248061	0.063987
H	3.150743	1.258993	0.944178
C	2.051224	2.557477	-0.491194
H	1.780610	2.473854	-1.552049
H	1.153875	2.941220	0.027126
H	2.822850	3.331122	-0.395912

1e-TS

C	-0.589210	-0.744192	0.725069
C	-1.288436	-2.048922	0.351602
C	-2.625572	-1.392544	-0.035691
C	-2.037397	-0.030058	-0.413568
C	-2.618839	1.191026	-0.052865
H	-1.323730	-2.797903	1.153487
H	-0.823997	-2.520806	-0.520693
H	-3.282441	-1.287772	0.836989
H	-3.199123	-1.883913	-0.832107
H	-1.483407	-0.029784	-1.356311
H	-0.894196	-0.366052	1.701728
C	0.782427	-0.385162	0.370305
C	1.446565	0.633183	1.093990
C	1.479365	-0.973091	-0.709720
C	2.735432	1.041257	0.759602
H	0.934787	1.100694	1.932986
C	2.771138	-0.565578	-1.042268
H	1.009848	-1.759745	-1.293688
C	3.408809	0.443765	-0.312945
H	3.219987	1.823755	1.338955
H	3.284544	-1.040347	-1.875258
H	4.416027	0.758009	-0.573758
H	-3.347192	1.196701	0.759947
C	-2.182138	2.522004	-0.584376
H	-3.042872	3.128941	-0.901238
H	-1.651117	3.115208	0.177413
H	-1.509983	2.412892	-1.443265

1f

C	3.274840	0.193188	0.264572
C	2.350902	0.226351	1.313068

C	1.022483	-0.148244	1.095706
C	0.584090	-0.565381	-0.172400
C	1.527677	-0.595809	-1.213336
C	2.857013	-0.221434	-1.002884
C	-0.844811	-0.947772	-0.447696
C	-2.012364	0.167973	-0.522296
C	-2.948108	-0.899059	0.125956
C	-1.710511	-1.702756	0.595605
H	-1.432654	-1.450811	1.624312
H	-1.740549	-2.794611	0.507484
H	-3.632329	-0.533154	0.899236
H	-3.532394	-1.437998	-0.628009
H	-0.880421	-1.493393	-1.398530
H	0.323022	-0.114614	1.926332
H	1.213938	-0.921380	-2.203610
H	2.664612	0.543384	2.304921
H	3.565443	-0.258119	-1.827096
H	4.308704	0.482869	0.434830
C	-1.825491	1.406029	0.269514
H	-2.246028	0.430539	-1.563145
C	-1.202324	2.634797	-0.309026
H	-1.458840	3.530777	0.269481
H	-0.099662	2.570466	-0.326724
H	-1.520923	2.796032	-1.348559
H	-1.972307	1.362716	1.348376

1f-TS

C	3.214549	0.339793	-0.466095
C	2.704365	0.900766	0.710675
C	1.447235	0.524843	1.179560
C	0.657321	-0.424403	0.493693
C	1.189194	-0.976351	-0.691597
C	2.448385	-0.600714	-1.161714
C	-0.676520	-0.760676	1.000826
C	-1.427699	-2.013640	0.533399
C	-2.300996	-1.314736	-0.524841
C	-2.170334	0.102938	0.042390
C	-1.915932	1.227313	-0.755740
C	-1.986955	2.639163	-0.261180
H	-0.814883	-0.477296	2.044579
H	-2.033267	-2.420883	1.351386
H	-0.789097	-2.825038	0.163831

H	-3.334236	-1.674653	-0.616793
H	-1.842279	-1.362435	-1.519766
H	-2.791001	0.290050	0.922934
H	1.063277	0.964226	2.098370
H	0.616346	-1.711677	-1.250162
H	3.290941	1.629096	1.265856
H	2.834166	-1.047002	-2.075443
H	4.196088	0.628815	-0.832738
H	-2.511268	2.705904	0.699814
H	-0.982987	3.072164	-0.123241
H	-2.508000	3.290479	-0.977482
H	-1.489481	1.072476	-1.747395

1g

C	-3.651674	-0.614585	0.179454
C	-3.023830	0.233424	1.097694
C	-1.725721	0.689559	0.861116
C	-1.022331	0.312505	-0.296134
C	-1.668179	-0.538976	-1.207098
C	-2.967423	-0.999486	-0.975906
C	0.385367	0.778676	-0.553578
C	1.545862	0.397553	0.473742
C	2.318568	-0.863368	0.308061
C	2.126629	-1.996972	1.271500
C	2.173106	1.794258	0.158375
C	0.795276	2.267600	-0.367585
C	3.025510	-1.172180	-0.978482
H	0.206433	2.756720	0.416032
H	0.773881	2.900088	-1.261692
H	2.616614	2.333423	1.002428
H	2.915501	1.736016	-0.644855
H	1.115127	0.430907	1.482736
H	0.694280	0.448153	-1.552734
H	-1.255756	1.348097	1.588220
H	-1.145281	-0.842537	-2.112152
H	-3.546793	0.541023	2.000229
H	-3.444137	-1.656249	-1.699786
H	-4.662867	-0.968924	0.362936
H	2.433102	-1.852681	-1.618326
H	3.237035	-0.277112	-1.573866
H	3.981103	-1.685302	-0.796613
H	3.049189	-2.582483	1.396098

H	1.809806	-1.647015	2.261331
H	1.355805	-2.710169	0.923053

1g-TS

C	3.659562	-0.699420	0.197111
C	2.852668	-1.282288	-0.788023
C	1.597119	-0.751284	-1.071931
C	1.099240	0.380606	-0.383314
C	1.929549	0.952091	0.608061
C	3.188094	0.420970	0.889897
C	-0.244921	0.869692	-0.677326
C	-0.780369	2.255835	-0.330629
C	-2.162821	1.767362	0.139377
C	-1.696905	0.374376	0.576211
C	-2.370574	-0.843494	0.374984
C	-3.421841	-1.054266	-0.679032
C	-1.901338	-2.087701	1.079656
H	-0.649440	0.483398	-1.614495
H	-0.773401	2.975909	-1.159524
H	-0.227595	2.704422	0.501649
H	-2.858149	1.710321	-0.704443
H	-2.645159	2.354598	0.931720
H	-1.093012	0.405242	1.486459
H	0.980878	-1.210080	-1.842864
H	1.589999	1.823058	1.161401
H	3.207409	-2.150403	-1.338832
H	3.806212	0.885989	1.654525
H	4.641170	-1.110152	0.418490
H	-1.150785	-1.868730	1.846402
H	-2.740007	-2.612803	1.562236
H	-1.455006	-2.808316	0.374480
H	-3.794153	-0.122567	-1.114054
H	-3.038647	-1.677056	-1.505860
H	-4.285086	-1.597700	-0.267542

1h

C	-2.575918	-0.615883	0.670137
O	-2.304487	-0.694539	1.862310
O	-3.582594	-1.411747	0.196372
C	-3.942756	-1.418593	-1.186563

H	-3.097739	-1.711341	-1.820860
H	-4.733358	-2.165538	-1.275783
H	-4.332091	-0.444461	-1.506192
C	-1.883992	0.288367	-0.235430
H	-2.193666	0.372156	-1.273517
C	-0.768754	1.134362	0.222020
C	0.560620	1.164490	-0.638719
C	-0.846162	2.687145	0.008187
H	-0.539654	0.912361	1.267369
C	0.668050	2.683287	-0.312036
H	0.288210	1.049755	-1.695784
H	-1.449800	2.941336	-0.870859
H	-1.198550	3.274035	0.861888
H	1.029996	3.338047	-1.111341
H	1.272666	2.857699	0.584374
C	1.687578	0.218288	-0.317050
C	2.217295	0.118753	0.980189
C	2.243437	-0.589074	-1.321372
C	3.266807	-0.757024	1.262289
H	1.803648	0.724845	1.782917
C	3.295930	-1.466348	-1.045118
H	1.848408	-0.527446	-2.333847
C	3.811677	-1.553402	0.249823
H	3.657255	-0.820788	2.274923
H	3.710058	-2.080565	-1.841028
H	4.628396	-2.236010	0.470155

1h-TS

C	2.239937	-0.818890	-0.621216
O	1.506806	-1.306329	-1.467557
O	3.301301	-1.577413	-0.195939
C	4.239987	-1.086916	0.761653
H	3.765263	-0.894073	1.731506
H	4.978040	-1.882764	0.878616
H	4.743061	-0.180007	0.405779
C	2.047433	0.515124	-0.052075
H	2.700187	0.874468	0.737502
C	0.973299	1.310757	-0.457819
C	-0.638592	1.291268	0.738558
C	0.840794	2.794052	-0.118437
H	0.469082	0.986442	-1.367666
C	-0.638620	2.751687	0.303167

H	-0.147279	1.129068	1.698078
H	1.488395	3.052558	0.728344
H	1.084970	3.467546	-0.949486
H	-0.939680	3.456326	1.088991
H	-1.290748	2.915944	-0.560000
C	-1.666760	0.306278	0.432592
C	-2.606211	0.473152	-0.609901
C	-1.719198	-0.893541	1.179870
C	-3.555271	-0.509498	-0.882515
H	-2.594239	1.376486	-1.212621
C	-2.665745	-1.875455	0.904180
H	-1.001108	-1.047068	1.982456
C	-3.591006	-1.688478	-0.129513
H	-4.268617	-0.357857	-1.688704
H	-2.682841	-2.789394	1.492335
H	-4.329643	-2.454976	-0.348426

2a

C	-1.953013	-0.000083	0.152281
C	-0.584199	0.000064	-0.402045
C	0.451781	1.080548	0.082265
C	1.562025	-0.000060	0.035212
C	0.451628	-1.080517	0.081976
H	2.089336	0.000017	-0.925741
H	2.305484	-0.000189	0.839259
H	0.563985	1.974664	-0.541109
H	0.232924	1.393637	1.110033
H	-0.615376	0.000305	-1.498704
H	0.232725	-1.393801	1.109672
H	-2.836271	0.001377	-0.479571
H	-2.105927	-0.001202	1.229587
H	0.563795	-1.974523	-0.541555

2a-TS

C	0.809207	1.159157	-0.139372
C	1.532276	-0.167914	0.006915
C	0.289968	-1.071649	-0.094434
C	-0.751760	-0.083256	0.433261
C	-1.985489	0.132034	-0.150687
H	0.983364	1.974319	0.561382

H	0.545821	1.477547	-1.146476
H	1.993515	-0.249452	0.998579
H	2.314047	-0.360453	-0.740001
H	0.334960	-2.015778	0.465761
H	0.068393	-1.314017	-1.141477
H	-0.663530	0.143955	1.497378
H	-2.740441	0.748699	0.329903
H	-2.201337	-0.215052	-1.159144

2b

C	-1.985529	0.383346	-0.081338
C	-0.798615	-0.339887	0.416025
C	-0.069886	-1.363466	-0.514088
C	1.290873	-0.898317	0.063360
C	0.606483	0.399082	0.580833
H	1.634541	-1.541473	0.881546
H	2.118273	-0.767145	-0.644017
H	-0.347133	-2.416742	-0.395279
H	-0.184674	-1.093985	-1.570389
H	-1.030851	-0.820799	1.374591
H	-2.825500	0.618655	0.566241
H	-2.019457	0.765734	-1.098552
H	0.833442	0.667359	1.620296
C	0.819527	1.617102	-0.314466
H	0.167786	2.449175	-0.021610
H	1.859683	1.961312	-0.245797
H	0.616774	1.390750	-1.368979

2b-TSI

C	0.711340	-1.366563	0.624646
C	1.503135	-0.363306	-0.193146
C	0.332225	0.569689	-0.585993
C	-0.790922	-0.480728	-0.497889
C	-2.022575	-0.301430	0.101368
H	0.791930	-2.434109	0.427423
H	0.485733	-1.116474	1.658967
H	1.935737	-0.842769	-1.079302
H	2.320348	0.135908	0.346472
H	0.418360	0.962269	-1.610482
H	-0.742532	-1.234529	-1.285770

H	-2.805374	-1.048577	0.000902
H	-2.218567	0.521687	0.783035
C	0.169045	1.753648	0.370128
H	1.037483	2.419508	0.296164
H	-0.725074	2.342370	0.133248
H	0.088469	1.426863	1.414661

2b-TSII

C	-0.932969	-0.209170	0.578315
C	-0.936250	1.222370	0.052873
C	0.505606	1.232963	-0.490856
C	1.090283	0.134647	0.399939
C	1.889548	-0.895428	-0.066436
H	-1.149522	-0.360761	1.636986
H	-1.057025	1.941848	0.871613
H	-1.715919	1.432703	-0.692722
H	1.034140	2.193539	-0.421091
H	0.536263	0.915240	-1.540226
H	1.225941	0.423004	1.444083
H	2.399819	-1.570707	0.615608
H	1.947301	-1.132069	-1.126799
C	-1.391804	-1.319177	-0.323569
H	-1.053255	-2.297641	0.037710
H	-2.492893	-1.349466	-0.378314
H	-1.021334	-1.192923	-1.348448

2c

C	1.735498	-1.218539	-0.147664
C	0.726571	-0.269049	0.361369
C	0.909632	1.268523	0.120971
C	-0.619915	1.392975	-0.090375
C	-0.666069	-0.131446	-0.377150
H	-1.139357	1.638670	0.844644
H	-0.976714	2.069828	-0.874506
H	1.372701	1.844365	0.929645
H	1.465630	1.454935	-0.805515
H	0.532904	-0.449513	1.427432
H	-0.507024	-0.307235	-1.449978
H	2.093351	-2.057514	0.441933
H	2.116770	-1.119596	-1.161959

C	-1.839510	-0.964547	0.117617
H	-2.764031	-0.703509	-0.414522
H	-1.656994	-2.036187	-0.035046
H	-2.014481	-0.801752	1.189268

2c- TSI

C	-0.867192	1.566832	0.041682
C	0.630092	1.358261	-0.071447
C	0.603471	-0.160368	-0.340501
C	-0.713256	-0.480992	0.376836
C	-1.705263	-1.290915	-0.140227
H	-1.298779	2.095700	0.889615
H	-1.435801	1.649222	-0.882666
H	1.123748	1.567622	0.886810
H	1.132911	1.958152	-0.842357
H	0.445815	-0.325178	-1.416268
H	-0.664600	-0.390768	1.464721
H	-2.556361	-1.600733	0.460526
H	-1.726113	-1.553408	-1.196205
C	1.817082	-0.970815	0.119720
H	1.675269	-2.040811	-0.075171
H	2.726833	-0.647298	-0.402498
H	1.987473	-0.844513	1.197113

2c-TSII

C	-0.881158	-0.107914	-0.457577
C	-0.624079	1.329705	-0.036736
C	0.906054	1.215063	0.083512
C	0.986559	-0.275475	0.415647
C	1.895506	-1.152149	-0.149821
H	-1.076161	1.525814	0.944668
H	-0.991450	2.098645	-0.730968
H	1.378867	1.868335	0.829373
H	1.390704	1.405327	-0.882510
H	0.599508	-0.538346	1.403001
H	2.006712	-2.169160	0.217041
H	2.448766	-0.889575	-1.049274
C	-1.988615	-0.931622	0.130980
H	-2.971944	-0.631637	-0.271392
H	-1.859817	-1.997466	-0.095319

H	-2.042028	-0.816261	1.221504
H	-0.648758	-0.321331	-1.502157

2d

C	-1.778468	1.304982	1.317847
C	-2.069043	-0.071009	0.863511
C	-3.106507	-0.178523	-0.294878
C	-1.949960	-0.339455	-1.312933
C	-1.006805	-0.745824	-0.149347
H	-1.665980	0.621077	-1.755536
H	-2.072219	-1.067767	-2.122448
H	-1.083200	-1.828817	0.005686
H	-3.714269	-1.086230	-0.211982
H	-3.776495	0.678272	-0.425341
H	-2.254744	-0.717698	1.731295
H	-2.047909	2.169533	0.716227
H	-1.165689	1.482268	2.197019
C	0.447387	-0.360836	-0.126067
C	0.899834	0.893191	-0.569612
C	1.401232	-1.261902	0.375211
C	2.253582	1.233007	-0.512775
H	0.190522	1.614414	-0.965856
C	2.756559	-0.927438	0.436402
H	1.075942	-2.241712	0.720412
C	3.188880	0.324553	-0.008375
H	2.578186	2.209548	-0.864369
H	3.473149	-1.646101	0.826965
H	4.242553	0.588741	0.034020

2d- TSI

C	-2.685691	-0.994040	0.355703
C	-1.962586	-1.040624	-0.978252
C	-1.100377	0.241061	-0.842050
C	-1.983822	0.958865	0.210364
C	-1.533259	1.562350	1.365205
H	-3.773050	-1.029178	0.396470
H	-2.190114	-1.414984	1.227341
H	-2.673645	-0.928937	-1.804701
H	-1.387568	-1.956661	-1.165179
H	-1.087047	0.830567	-1.769093

H	-2.920558	1.332934	-0.205764
H	-2.205990	2.155034	1.979568
H	-0.535912	1.380614	1.755067
C	0.345072	0.033617	-0.423588
C	0.763534	-1.041240	0.376648
C	1.315968	0.961020	-0.834725
C	2.102569	-1.182887	0.752693
H	0.044408	-1.782607	0.712985
C	2.655394	0.825464	-0.462359
H	1.015866	1.801825	-1.457043
C	3.055073	-0.249911	0.335710
H	2.399890	-2.026116	1.371622
H	3.385749	1.557208	-0.799240
H	4.096718	-0.361747	0.625871

2d-TSII

C	0.967510	-0.007744	-1.009969
C	1.942387	-1.182329	-0.863578
C	2.637454	-0.670249	0.410918
C	2.250145	0.803514	0.242835
C	1.769497	1.596018	1.292387
H	1.061894	0.589264	-1.917278
H	2.632012	-1.211634	-1.715036
H	1.472029	-2.169838	-0.788378
H	3.718078	-0.850307	0.482344
H	2.170028	-1.077895	1.315296
H	2.839488	1.332928	-0.509360
H	1.668438	2.672863	1.185763
H	1.340334	1.147671	2.185329
C	-0.413193	-0.079785	-0.519228
C	-0.853934	-1.060278	0.394320
C	-1.349313	0.892240	-0.934234
C	-2.168257	-1.069936	0.863655
H	-0.166151	-1.827788	0.738108
C	-2.661265	0.884409	-0.465283
H	-1.034625	1.659762	-1.638688
C	-3.080188	-0.098922	0.438491
H	-2.482053	-1.840985	1.563452
H	-3.360730	1.643546	-0.807331
H	-4.103793	-0.109212	0.803893

2e

C	-2.429293	1.642021	0.998859
C	-2.013859	0.274666	0.640267
C	-2.989777	-0.661832	-0.134636
C	-1.790820	-1.214675	-0.943338
C	-0.984300	0.060828	-0.568790
H	-1.368628	-2.113515	-0.480925
H	-1.933694	-1.410025	-2.011510
H	-3.579596	-1.365505	0.462420
H	-3.673040	-0.080503	-0.765483
H	-1.608828	-0.248979	1.515406
H	-1.178834	0.841603	-1.313691
H	-2.026394	2.152593	1.868784
H	-3.056367	2.219711	0.323162
C	0.491442	0.007755	-0.281969
C	1.050080	-0.988403	0.537262
C	1.353053	0.981204	-0.812456
C	2.418542	-1.011477	0.813334
H	0.411271	-1.757237	0.966361
C	2.723584	0.963808	-0.539209
H	0.942677	1.762758	-1.448925
C	3.262685	-0.034485	0.275721
H	2.826827	-1.793963	1.448637
H	3.368286	1.729349	-0.964367
H	4.328297	-0.052745	0.489851

2e-TSI

C	-3.077400	-0.975285	-0.315639
C	-1.690821	-1.541642	-0.095039
C	-1.014222	-0.244964	0.407289
C	-1.917866	0.764620	-0.314405
C	-2.468126	1.879276	0.282696
H	-3.596963	-1.120825	-1.260519
H	-3.725634	-0.865692	0.551220
H	-1.245324	-1.859289	-1.045390
H	-1.641596	-2.390980	0.598996
H	-1.219242	-0.148376	1.484686
H	-1.790888	0.787433	-1.398427
H	-3.003477	2.626178	-0.297640
H	-2.482856	1.991514	1.365041

C	0.483108	-0.096686	0.185067
C	1.324312	-1.220389	0.219538
C	1.067393	1.161868	-0.025617
C	2.705846	-1.092137	0.051507
H	0.898802	-2.207855	0.381431
C	2.448320	1.293672	-0.196085
H	0.434527	2.044804	-0.058105
C	3.274375	0.167098	-0.157908
H	3.336654	-1.977438	0.082527
H	2.878067	2.279083	-0.360338
H	4.348411	0.268858	-0.291908

2e-TSII

C	0.892879	-0.109245	0.710455
C	1.789028	-1.344770	0.713469
C	2.981261	-0.659238	0.022198
C	2.157002	0.402839	-0.713130
C	2.525313	1.748479	-0.794417
H	1.160463	0.610312	1.484822
H	1.382065	-2.141104	0.081735
H	1.977804	-1.772047	1.706740
H	3.599116	-1.292013	-0.627426
H	3.642164	-0.178259	0.753927
H	1.579121	0.014639	-1.554909
H	2.002503	2.438950	-1.450633
H	3.256202	2.173604	-0.109558
C	-0.528408	-0.089901	0.369107
C	-1.152146	-1.102656	-0.393426
C	-1.323255	1.010593	0.765461
C	-2.502327	-1.020126	-0.733220
H	-0.578854	-1.965548	-0.720693
C	-2.670915	1.093454	0.423508
H	-0.866279	1.804767	1.352255
C	-3.271068	0.076635	-0.328838
H	-2.957987	-1.817354	-1.315845
H	-3.257262	1.950234	0.746972
H	-4.323239	0.137433	-0.594391

2f

C	-1.377402	1.580037	-0.378566

C	-1.152601	0.426291	0.529265
C	-1.721569	-0.947362	0.008639
C	-0.297060	-1.317381	-0.485794
C	0.259360	-0.217234	0.457637
H	-0.150845	-1.032840	-1.533543
H	0.045367	-2.347033	-0.336740
H	0.541467	-0.643853	1.434492
H	-2.061948	-1.587019	0.830332
H	-2.510148	-0.889802	-0.747302
H	-1.480637	0.675034	1.552121
H	-2.389519	1.938370	-0.548497
H	-0.550201	2.123080	-0.821253
O	1.286049	0.632662	0.000304
C	2.553289	0.001773	-0.062242
H	3.269253	0.756065	-0.398446
H	2.860927	-0.372954	0.927233
H	2.553791	-0.837095	-0.774464

2f- TSI

C	1.506851	-1.688551	-0.140882
C	1.211346	-0.488786	0.472553
C	-0.200562	0.086327	0.612869
O	-1.058013	-0.561428	-0.316017
C	-2.430313	-0.265340	-0.133894
C	1.324976	1.253532	-0.659531
C	0.120165	1.542465	0.214360
H	0.401269	2.125918	1.099584
H	-0.706578	2.066508	-0.282742
H	2.261732	1.787239	-0.509740
H	1.137900	0.928495	-1.679534
H	1.898484	-0.127622	1.238306
H	2.509791	-2.103864	-0.094364
H	0.779819	-2.185846	-0.774335
H	-0.616588	-0.037278	1.628432
H	-2.979333	-0.842944	-0.882024
H	-2.769545	-0.560535	0.871682
H	-2.647629	0.803463	-0.279977

2f-TSII

C	0.344685	-0.680580	0.521215

C	-0.807201	-1.547721	0.052260
C	-1.705495	-0.403887	-0.453989
C	-1.130325	0.722593	0.411136
C	-0.825017	1.985787	-0.079471
H	0.728393	-0.762540	1.545493
H	-1.256541	-2.069455	0.905568
H	-0.517232	-2.296363	-0.694907
H	-2.786543	-0.554903	-0.332930
H	-1.510110	-0.194376	-1.511736
H	-1.409030	0.665894	1.466646
H	-0.587501	2.811368	0.586935
H	-0.711877	2.163882	-1.146526
O	1.321820	-0.516325	-0.424313
C	2.376768	0.361562	-0.043223
H	3.104675	0.349693	-0.857136
H	1.995284	1.379369	0.102191
H	2.855427	0.011506	0.883330

2g

C	-1.917762	-1.489623	0.199147
C	-1.140375	-0.359556	-0.349653
C	-1.558972	1.113055	-0.028249
C	-0.059215	1.504726	0.042419
C	0.257795	0.000434	0.255893
H	0.317443	1.841011	-0.930219
H	0.251580	2.214212	0.816272
H	-2.184867	1.618754	-0.769776
H	-2.049381	1.182246	0.949648
H	-0.992506	-0.473633	-1.430792
H	0.296238	-0.251045	1.328758
H	-2.012219	-2.430783	-0.333946
H	-2.330241	-1.436423	1.204311
O	1.345263	-0.587252	-0.417672
C	2.604040	-0.267027	0.152024
H	2.660789	-0.594868	1.202186
H	3.361616	-0.797229	-0.430660
H	2.806372	0.813709	0.106100

2g- TSI

C	1.553771	1.414828	0.068020

C	0.042767	1.471722	0.001644
C	-0.199599	-0.036714	0.213187
C	1.089591	-0.585412	-0.378640
C	1.843245	-1.579629	0.209695
H	2.164358	1.848978	-0.719933
H	2.022323	1.385321	1.049143
H	-0.297779	1.759002	-1.000358
H	-0.434281	2.135307	0.734090
H	-0.229725	-0.265418	1.292733
H	1.173525	-0.448771	-1.457141
H	2.684088	-2.034291	-0.306686
H	1.680505	-1.874816	1.244013
O	-1.331002	-0.610166	-0.421141
C	-2.565518	-0.222828	0.157522
H	-3.350782	-0.761383	-0.379018
H	-2.607826	-0.493292	1.224910
H	-2.741930	0.858887	0.058801

2g-TSII

C	1.546345	1.806271	0.117505
C	1.173311	0.582604	-0.421447
C	-0.435782	-0.427027	0.357332
O	-1.645138	-0.426391	-0.283594
C	-2.506562	0.655941	0.059385
C	1.782184	-0.754008	0.007387
C	0.485229	-1.582849	0.047801
H	0.240199	-1.972956	-0.946988
H	0.456575	-2.419529	0.758993
H	2.562986	-1.132189	-0.664755
H	2.222844	-0.658224	1.007838
H	0.785298	0.590417	-1.443171
H	-0.475376	-0.072360	1.393072
H	1.211908	2.744327	-0.317954
H	2.096002	1.866865	1.054682
H	-2.063537	1.613588	-0.241492
H	-3.442045	0.495545	-0.480241
H	-2.702109	0.670053	1.140992

2h

C	-0.682018	1.990073	0.431870

C	-1.121184	0.803278	-0.325813
C	-0.071407	-0.342629	-0.781615
C	-1.141957	-1.396847	-0.407678
C	-1.909916	-0.327785	0.405629
H	-1.695710	-1.737374	-1.288984
H	-0.774620	-2.262718	0.148906
H	0.205705	-0.264987	-1.839140
H	-1.653290	1.109883	-1.233618
H	-1.648566	-0.366953	1.467800
H	-0.689138	2.983477	-0.007345
H	-0.300568	1.888880	1.444961
H	-3.000240	-0.289643	0.308151
C	1.180841	-0.361664	0.072533
C	2.365247	0.433066	-0.445266
H	3.151038	0.476522	0.312488
H	2.762613	-0.042482	-1.352304
H	2.056686	1.448710	-0.723356
O	1.233558	-0.966032	1.133060

2h- TSI

C	-0.682018	1.990073	0.431870
C	-1.121184	0.803278	-0.325813
C	-0.071407	-0.342629	-0.781615
C	-1.141957	-1.396847	-0.407678
C	-1.909916	-0.327785	0.405629
H	-1.695710	-1.737374	-1.288984
H	-0.774620	-2.262718	0.148906
H	0.205705	-0.264987	-1.839140
H	-1.653290	1.109883	-1.233618
H	-1.648566	-0.366953	1.467800
H	-0.689138	2.983477	-0.007345
H	-0.300568	1.888880	1.444961
H	-3.000240	-0.289643	0.308151
C	1.180841	-0.361664	0.072533
C	2.365247	0.433066	-0.445266
H	3.151038	0.476522	0.312488
H	2.762613	-0.042482	-1.352304
H	2.056686	1.448710	-0.723356
O	1.233558	-0.966032	1.133060

2h-TSII

C	-0.079576	-0.497688	-0.805345
C	1.022230	-1.467040	-0.385447
C	1.868603	-0.432651	0.379442
C	1.313263	0.817321	-0.312767
C	0.939071	1.980963	0.368693
H	-0.277182	-0.344181	-1.866345
H	1.547398	-1.863885	-1.261202
H	0.659233	-2.302727	0.220381
H	2.957954	-0.535420	0.295404
H	1.602023	-0.422232	1.441041
H	1.682611	0.969340	-1.329134
H	0.724712	2.903762	-0.164179
H	0.742104	1.966757	1.437931
C	-1.246662	-0.317361	0.079165
C	-2.381868	0.548395	-0.440558
H	-2.006927	1.544485	-0.710870
H	-2.821057	0.110921	-1.346512
H	-3.154712	0.646394	0.325232
O	-1.283315	-0.808106	1.207395

2i

C	1.488840	1.890465	-0.192336
C	1.099596	0.493514	-0.445282
C	2.061901	-0.671528	-0.041126
C	0.846253	-1.507488	0.426053
C	0.014462	-0.210107	0.512369
H	0.457355	-2.158526	-0.362278
H	0.952103	-2.086972	1.348448
H	2.692344	-1.076425	-0.839782
H	2.703770	-0.372659	0.795947
H	0.770496	0.357219	-1.481940
H	0.066665	0.256292	1.503362
H	1.292717	2.683223	-0.908203
H	1.957590	2.167096	0.749512
C	-1.403522	-0.189284	-0.013331
C	-2.253350	1.007901	0.370370
H	-2.513492	0.947763	1.436004
H	-1.694067	1.942274	0.232764
H	-3.171551	1.027566	-0.221455
O	-1.829876	-1.070961	-0.744085

2i- TSI

C	1.488840	1.890465	-0.192336
C	1.099596	0.493514	-0.445282
C	2.061901	-0.671528	-0.041126
C	0.846253	-1.507488	0.426053
C	0.014462	-0.210107	0.512369
H	0.457355	-2.158526	-0.362278
H	0.952103	-2.086972	1.348448
H	2.692344	-1.076425	-0.839782
H	2.703770	-0.372659	0.795947
H	0.770496	0.357219	-1.481940
H	0.066665	0.256292	1.503362
H	1.292717	2.683223	-0.908203
H	1.957590	2.167096	0.749512
C	-1.403522	-0.189284	-0.013331
C	-2.253350	1.007901	0.370370
H	-2.513492	0.947763	1.436004
H	-1.694067	1.942274	0.232764
H	-3.171551	1.027566	-0.221455
O	-1.829876	-1.070961	-0.744085

2i-TSII

C	-0.117715	-0.280860	0.629491
C	0.775152	-1.498984	0.442112
C	2.021865	-0.710194	0.004133
C	1.276798	0.527071	-0.511702
C	1.643058	1.838474	-0.199378
H	-0.012172	0.253838	1.573447
H	0.380607	-2.119368	-0.368101
H	0.891302	-2.121775	1.336649
H	2.660697	-1.189271	-0.747994
H	2.650100	-0.439264	0.861508
H	0.777770	0.378282	-1.470677
H	1.194300	2.688110	-0.706999
H	2.310748	2.053441	0.632129
C	-1.432647	-0.163577	-0.022847
C	-2.327877	0.978887	0.428914
H	-2.722822	0.772332	1.432755
H	-1.765666	1.919419	0.492119
H	-3.165125	1.092981	-0.263686

O	-1.778944	-0.929203	-0.924435

3a

C	-1.153838	-1.279554	-0.141789
C	-0.679028	0.013436	-0.844455
C	-1.096376	1.331628	-0.158086
C	0.157184	1.284023	0.761159
C	0.680455	-0.014386	0.070498
C	0.144409	-1.329144	0.712981
C	2.033069	-0.008103	-0.470752
H	-1.092387	2.189894	-0.838576
H	-2.069559	1.303820	0.347389
H	-0.039974	1.170839	1.834051
H	0.830494	2.138077	0.629217
H	-0.637017	0.002737	-1.937087
H	0.013946	-1.284420	1.801155
H	0.777140	-2.193409	0.481967
H	-1.261507	-2.133236	-0.819155
H	-2.090337	-1.173838	0.419521
H	2.518699	-0.931927	-0.776690
H	2.535256	0.924072	-0.719127

3a-TSI

C	1.010045	-0.931773	0.976471
C	1.667152	-0.374606	-0.278494
C	0.447501	0.348743	-0.854841
C	-0.705677	-0.342082	-0.065540
C	-1.518324	-1.401659	-0.403196
C	0.063537	1.685032	-0.140151
C	-1.090548	0.972123	0.633043
H	1.986742	-1.188421	-0.940829
H	2.539573	0.269738	-0.098724
H	1.013147	-0.325011	1.880833
H	1.014330	-2.004025	1.156571
H	0.380838	0.374130	-1.949530
H	-1.012668	0.984792	1.725120
H	-2.092443	1.323423	0.358641
H	-0.278331	2.468512	-0.823286
H	0.857104	2.102162	0.490204
H	-2.434069	-1.607051	0.147473

H	-1.216332	-2.132920	-1.150227

3a-TSII

C	-0.193219	1.298211	0.699660
C	1.133471	1.297711	-0.101096
C	0.843990	0.000034	-0.852932
C	1.133624	-1.297572	-0.101026
C	-0.193210	-1.298354	0.699495
C	-0.772675	-0.000035	0.092853
C	-2.043395	0.000000	-0.507931
H	1.216251	-2.158974	-0.772109
H	2.047242	-1.261039	0.509021
H	-0.084099	-1.245686	1.791276
H	-0.822920	-2.164524	0.468662
H	0.882852	-0.000008	-1.942861
H	-0.083874	1.245269	1.791404
H	-0.823047	2.164391	0.469186
H	1.215712	2.159112	-0.772229
H	2.047229	1.261441	0.508760
H	-2.523442	0.927221	-0.812544
H	-2.523417	-0.927179	-0.812703

3b

C	-0.531160	-0.058974	-0.632971
C	-1.279482	1.252148	-1.015970
C	-2.409386	0.946646	-0.019130
C	-3.475068	-0.072082	-0.497635
C	-2.716702	-1.231773	0.206927
C	-1.536559	-0.287054	0.583538
C	-1.018206	-0.334960	1.944256
H	-4.481615	0.108844	-0.107277
H	-3.546790	-0.158138	-1.588696
H	-2.445789	-2.099053	-0.408062
H	-3.241667	-1.594977	1.097799
H	-2.759711	1.762678	0.618947
H	-0.708086	-0.841952	-1.380047
H	-0.721231	2.150446	-0.734846
H	-1.567319	1.349044	-2.070469
H	-0.031306	0.037416	2.200179
H	-1.664583	-0.647415	2.760987

C	0.955321	-0.018740	-0.363757
C	1.742956	-1.141052	-0.671861
C	1.596901	1.090427	0.211347
C	3.116235	-1.159468	-0.418278
H	1.270527	-2.012312	-1.121534
C	2.971124	1.079108	0.466521
H	1.024518	1.977865	0.467868
C	3.737991	-0.045984	0.153174
H	3.700013	-2.041234	-0.671649
H	3.442023	1.952944	0.910704
H	4.807239	-0.053608	0.349120

3b-TSI

C	0.439694	-0.013766	-0.735067
C	1.268183	-1.274409	-0.986762
C	2.436508	-0.901384	-0.072205
C	3.406567	0.193042	-0.619646
C	2.710446	1.285295	0.252447
C	1.729667	0.211320	0.762131
C	1.177005	0.141475	2.040852
H	4.456119	0.022731	-0.361440
H	3.342559	0.351317	-1.702458
H	2.272749	2.129969	-0.291598
H	3.350977	1.687243	1.046145
H	2.921325	-1.731640	0.454159
H	0.732319	0.835064	-1.354249
H	0.760076	-2.171070	-0.616699
H	1.519134	-1.449408	-2.042628
H	0.779591	-0.789689	2.437959
H	0.986279	1.043526	2.618396
C	-0.994014	-0.012365	-0.433348
C	-1.744808	1.166028	-0.643167
C	-1.669734	-1.124183	0.112252
C	-3.101371	1.230025	-0.332281
H	-1.248402	2.038821	-1.063084
C	-3.029122	-1.062367	0.421039
H	-1.130970	-2.048716	0.298389
C	-3.754226	0.113005	0.201843
H	-3.652863	2.150067	-0.510962
H	-3.524583	-1.936802	0.836485
H	-4.813082	0.158299	0.443055

3b-TSII

C	-0.534965	-0.120314	-0.596664
C	-1.252611	1.176572	-1.060236
C	-2.453529	1.043759	-0.137680
C	-3.479923	-0.030703	-0.498254
C	-2.752791	-1.173436	0.250730
C	-1.485383	-0.376658	0.632016
C	-1.012568	-0.392875	1.951615
H	-4.480370	0.175840	-0.104700
H	-3.575091	-0.185867	-1.582069
H	-2.540623	-2.078167	-0.336221
H	-3.296496	-1.478241	1.151744
H	-2.778218	1.909113	0.441051
H	-0.697759	-0.931892	-1.318157
H	-0.666691	2.068672	-0.818911
H	-1.489004	1.214840	-2.133886
H	-0.034650	-0.006455	2.220816
H	-1.668523	-0.691413	2.765959
C	0.955144	-0.046690	-0.337558
C	1.779576	-1.117262	-0.719929
C	1.561309	1.053251	0.291739
C	3.156759	-1.095371	-0.485877
H	1.334203	-1.980472	-1.210638
C	2.937846	1.080972	0.530125
H	0.957200	1.900283	0.606571
C	3.742855	0.006563	0.141842
H	3.770351	-1.937408	-0.797136
H	3.381104	1.944742	1.019996
H	4.814252	0.029577	0.324362

3c

C	-0.508499	-0.258697	-0.892950
C	-1.316229	-1.562731	-0.627540
C	-2.565056	-0.734627	-0.235021
C	-2.786606	-0.567929	1.278724
C	-1.700723	0.543848	1.325582
C	-1.638616	0.606187	-0.237637
C	-2.023237	1.857452	-0.879187
H	-3.784693	-0.179325	1.509799
H	-2.612764	-1.460320	1.892743

H	-0.754218	0.240612	1.784989
H	-2.018456	1.481353	1.793811
H	-3.437043	-0.823319	-0.888601
H	-0.533559	-0.048044	-1.972173
H	-1.436385	-2.220284	-1.494175
H	-0.931142	-2.162888	0.205515
H	-1.887382	1.999787	-1.949169
H	-2.585306	2.617911	-0.342365
C	0.917309	-0.120691	-0.408936
C	1.743657	-1.241552	-0.239805
C	1.461417	1.148974	-0.152513
C	3.073942	-1.101005	0.168992
H	1.348531	-2.235916	-0.433431
C	2.787870	1.293499	0.259004
H	0.835036	2.030134	-0.273166
C	3.601580	0.167355	0.420911
H	3.696018	-1.984637	0.291175
H	3.186267	2.286219	0.455185
H	4.634248	0.278221	0.742115

3c-TSI

C	0.424994	0.444285	1.018555
C	1.396742	-0.606013	1.564719
C	2.529761	-0.386554	0.543965
C	2.525941	-1.358216	-0.670828
C	1.603004	-0.382436	-1.467034
C	1.830389	0.670640	-0.367614
C	2.165767	2.002839	-0.597177
H	3.517576	-1.457348	-1.124435
H	2.127941	-2.361755	-0.479601
H	0.567755	-0.725388	-1.565214
H	1.964037	-0.091301	-2.459205
H	3.508380	-0.150982	0.976126
H	0.511008	1.409246	1.514141
H	1.690438	-0.386214	2.598684
H	1.002498	-1.627886	1.556522
H	2.644761	2.607778	0.170130
H	1.846723	2.513052	-1.503469
C	-0.925010	0.170523	0.536791
C	-1.388557	-1.126189	0.217587
C	-1.816769	1.249956	0.325195
C	-2.677881	-1.330991	-0.276093

H	-0.741746	-1.985239	0.370902
C	-3.099939	1.044799	-0.172904
H	-1.484752	2.258809	0.561553
C	-3.541247	-0.249884	-0.477052
H	-3.009892	-2.341332	-0.503376
H	-3.762913	1.894098	-0.320355
H	-4.544984	-0.412088	-0.861056

3c-TSII

C	-0.521159	-0.273967	-0.861275
C	-1.292396	-1.584118	-0.541119
C	-2.605185	-0.886975	-0.189402
C	-2.796795	-0.518329	1.274785
C	-1.764761	0.635220	1.263184
C	-1.583980	0.693767	-0.275658
C	-1.973191	1.838729	-0.986432
H	-3.810430	-0.147814	1.462665
H	-2.596353	-1.334249	1.984416
H	-0.826203	0.403342	1.779922
H	-2.146651	1.575539	1.674457
H	-3.471796	-1.041390	-0.832506
H	-0.537332	-0.130219	-1.951027
H	-1.361530	-2.277643	-1.385178
H	-0.877115	-2.135078	0.313384
H	-1.775193	1.934567	-2.051786
H	-2.602468	2.599775	-0.530611
C	0.912701	-0.123923	-0.384681
C	1.751686	-1.241793	-0.257073
C	1.449583	1.142592	-0.102747
C	3.085704	-1.100926	0.137465
H	1.364144	-2.234653	-0.472696
C	2.780805	1.287144	0.295301
H	0.815450	2.021082	-0.194265
C	3.605982	0.165025	0.416994
H	3.716638	-1.982154	0.227246
H	3.173107	2.278013	0.512007
H	4.641763	0.276220	0.727907

3d

C	0.348669	0.355919	-0.539822

C	-0.395599	1.629478	-0.073895
C	-1.525674	0.788839	0.541483
C	-2.598244	0.264014	-0.447842
C	-1.837874	-1.084082	-0.604338
C	-0.666153	-0.568222	0.275575
C	-0.158764	-1.419074	1.345827
H	-3.598636	0.163588	-0.015382
H	-2.684955	0.859463	-1.364658
H	-1.568134	-1.387397	-1.623279
H	-2.362178	-1.919954	-0.127024
H	-1.867536	1.051371	1.545998
H	0.259688	0.146885	-1.613296
H	0.192492	2.157634	0.682625
H	-0.686068	2.337818	-0.859092
H	0.723260	-1.146478	1.919261
H	-0.765211	-2.237920	1.724403
C	1.809214	0.223407	-0.142757
O	2.325422	0.955645	0.686490
C	2.592606	-0.888116	-0.815977
H	2.748828	-0.638012	-1.874276
H	3.563374	-1.014262	-0.330733
H	2.032615	-1.830869	-0.785984

3d-TSI

C	-0.468413	-0.472784	-0.589565
C	0.338409	-1.622364	0.001592
C	1.506509	-0.780824	0.520135
C	2.550970	-0.335902	-0.551765
C	1.883341	1.071142	-0.661361
C	0.860427	0.637055	0.405311
C	0.314190	1.446502	1.399961
H	3.578688	-0.304751	-0.177772
H	2.537269	-0.932114	-1.470907
H	1.480688	1.334405	-1.645144
H	2.522318	1.895762	-0.325052
H	1.924776	-1.083955	1.486106
H	-0.262223	-0.189720	-1.621744
H	-0.228146	-2.075191	0.821258
H	0.607486	-2.408284	-0.715862
H	-0.143196	1.018842	2.288423
H	0.215812	2.520646	1.255763
C	-1.850501	-0.218171	-0.142810

O	-2.322959	-0.764896	0.853249
C	-2.652704	0.803319	-0.932992
H	-2.829107	0.445086	-1.955801
H	-3.613096	0.981354	-0.443780
H	-2.100967	1.749247	-1.012523

3d-TSII

C	-0.332897	-0.331248	-0.509490
C	0.406055	-1.608433	-0.064374
C	1.611451	-0.896585	0.527493
C	2.595280	-0.257890	-0.455025
C	1.837827	1.089037	-0.568470
C	0.602272	0.674952	0.255296
C	0.128131	1.477653	1.302202
H	3.605411	-0.150649	-0.047381
H	2.675740	-0.812204	-1.400286
H	1.598439	1.422974	-1.587684
H	2.375220	1.901194	-0.066348
H	1.966880	-1.182132	1.517629
H	-0.254798	-0.133662	-1.587981
H	-0.177765	-2.120896	0.706041
H	0.632973	-2.324458	-0.867357
H	-0.794646	1.251610	1.829727
H	0.763164	2.247996	1.732513
C	-1.806962	-0.238986	-0.127237
O	-2.311814	-0.990329	0.690334
C	-2.616634	0.842902	-0.817092
H	-2.794274	0.550527	-1.861345
H	-3.579283	0.971260	-0.316352
H	-2.069695	1.792656	-0.833659

3e

C	0.469381	-0.065623	-0.811194
C	-0.479775	-1.241701	-1.136081
C	-1.704912	-0.427352	-0.650506
C	-2.165157	-0.714790	0.791418
C	-1.055920	0.222925	1.347369
C	-0.698696	0.724185	-0.092062
C	-0.843228	2.145725	-0.372217
H	-3.172752	-0.335284	0.993289

H	-2.120639	-1.764444	1.104145
H	-0.239644	-0.294545	1.860973
H	-1.418496	1.021989	2.002399
H	-2.462404	-0.187918	-1.401528
H	0.752291	0.495151	-1.711556
H	-0.499740	-1.528602	-2.191766
H	-0.274561	-2.134372	-0.536900
H	-0.536427	2.559869	-1.330182
H	-1.395454	2.798552	0.299095
C	1.710621	-0.318314	0.020788
C	2.644673	0.861938	0.216556
H	3.160189	1.084439	-0.727641
H	2.083149	1.763282	0.492473
H	3.388320	0.630853	0.983035
O	1.934281	-1.403866	0.534967

3e-TSI

C	-0.628116	-0.024945	0.917169
C	0.413734	-1.067632	1.304170
C	1.644052	-0.346988	0.714201
C	2.125300	-0.869839	-0.668070
C	1.124446	0.090040	-1.386301
C	0.904827	0.803336	-0.038456
C	0.959342	2.180483	0.163820
H	3.170125	-0.608331	-0.866265
H	1.983237	-1.939998	-0.850263
H	0.244228	-0.427283	-1.778038
H	1.541733	0.725552	-2.174438
H	2.418295	-0.080847	1.441526
H	-0.850048	0.733589	1.666018
H	0.468392	-1.226109	2.387196
H	0.210356	-2.030528	0.825640
H	1.146437	2.601216	1.149492
H	0.719247	2.876806	-0.636912
C	-1.720816	-0.314962	-0.016015
C	-2.801460	0.743845	-0.168289
H	-3.459409	0.737746	0.711187
H	-2.366091	1.748479	-0.239643
H	-3.402598	0.535620	-1.056756
O	-1.743970	-1.350742	-0.689015

3e-TSII

C	0.440951	-0.084684	-0.788140
C	-0.495440	-1.275097	-1.076622
C	-1.776411	-0.552112	-0.662588
C	-2.171978	-0.654855	0.804356
C	-1.090441	0.330975	1.311041
C	-0.620520	0.820494	-0.083542
C	-0.745000	2.170666	-0.437504
H	-3.183148	-0.271414	0.977729
H	-2.117073	-1.670894	1.218268
H	-0.289104	-0.143216	1.889802
H	-1.494397	1.151954	1.912457
H	-2.537520	-0.355565	-1.417752
H	0.738730	0.420729	-1.716048
H	-0.482962	-1.592697	-2.123724
H	-0.269012	-2.146710	-0.451744
H	-0.347056	2.548545	-1.376630
H	-1.367754	2.847984	0.141944
C	1.696846	-0.346783	0.036651
C	2.657939	0.815493	0.201851
H	3.154347	1.020023	-0.756616
H	2.122949	1.729910	0.484478
H	3.415288	0.571835	0.950798
O	1.910129	-1.431883	0.554253

4a

C	0.113763	-0.740040	0.585786
C	1.438854	-0.616746	-0.228389
C	1.216632	0.873844	-0.266351
C	-0.038489	0.832328	0.551925
C	-1.371912	0.669348	-0.260876
C	-1.175901	-0.876871	-0.270772
H	-2.250603	0.985734	0.312994
H	-1.396864	1.169690	-1.234916
H	-1.021222	-1.329107	-1.257580
H	-1.983675	-1.422819	0.228129
H	-0.098247	1.464783	1.446814
H	1.464664	-1.154411	-1.189950
H	1.697699	1.672767	-0.826822
H	2.334171	-0.925959	0.336297
H	0.156386	-1.311864	1.517095

4a-TSI

C	-1.390483	-0.680539	0.001807
C	0.025615	-0.686749	0.589675
C	1.218603	-0.786764	-0.434385
C	1.468797	0.682198	-0.162146
C	0.349158	0.827162	0.643014
C	-1.412068	0.759098	-0.494969
H	-2.133303	1.457958	-0.074191
H	-1.135396	0.967637	-1.526025
H	-1.568715	-1.438706	-0.773127
H	-2.139608	-0.832977	0.788724
H	0.098928	1.590125	1.377441
H	0.915520	-1.048217	-1.460092
H	2.207511	1.380489	-0.547815
H	2.022561	-1.475082	-0.137878
H	0.174769	-1.287668	1.494983

4a-TSII

C	1.314715	-0.770451	0.075508
C	-0.041243	-0.900874	-0.586925
C	-1.257559	-0.766604	0.346040
C	-1.350694	0.730681	0.172160
C	-0.094993	1.085836	-0.389742
C	1.238715	0.750107	0.331590
H	2.071954	1.285618	-0.136592
H	1.212573	1.044916	1.389202
H	1.431753	-1.389775	0.977853
H	2.129739	-1.023867	-0.610810
H	-0.052227	1.950920	-1.060079
H	-1.055846	-1.140540	1.361962
H	-2.276976	1.243007	-0.076941
H	-2.153318	-1.285605	-0.018925
H	-0.161303	-1.456846	-1.517455

4b

C	3.388880	-0.128214	-0.144209
C	2.795489	1.054876	0.304244

C	1.404600	1.151464	0.401058
C	0.577890	0.070140	0.055932
C	1.188962	-1.113491	-0.389734
C	2.578533	-1.213289	-0.491197
C	-0.914320	0.154800	0.208527
C	-1.540533	-0.565056	1.464905
C	-2.500340	-1.258192	0.537633
C	-1.954328	-0.628515	-0.704162
C	-2.612953	0.739169	-1.095087
C	-1.636433	1.491949	-0.146933
H	-2.458196	0.988701	-2.150655
H	-3.680857	0.826797	-0.869564
H	-2.100461	2.001904	0.705033
H	-0.996599	2.210071	-0.669057
H	-1.663244	-1.274062	-1.542323
H	-1.960832	0.104094	2.232879
H	-3.403943	-1.834368	0.722406
H	-0.828510	-1.236198	1.970984
H	0.957122	2.079326	0.750030
H	0.569439	-1.964585	-0.663338
H	3.414964	1.906033	0.577161
H	3.028078	-2.138342	-0.844501
H	4.470365	-0.203216	-0.224911

4b-TSI

C	-1.601101	1.477257	-0.330212
C	-0.938167	0.153872	0.110697
C	-1.541377	-0.461416	1.451112
C	-2.244987	-1.473708	0.574877
C	-1.841339	-0.886429	-0.609399
C	-2.894920	0.918353	-0.892870
C	0.565987	0.070809	0.006059
C	1.364308	1.153693	0.411717
C	2.758046	1.082149	0.355203
C	3.384351	-0.077268	-0.112138
C	2.602713	-1.160835	-0.520648
C	1.207959	-1.085760	-0.461726
H	-3.108474	1.033216	-1.953734
H	-3.774284	0.864886	-0.255770
H	-1.734206	2.209868	0.477126
H	-1.007946	1.956794	-1.117776
H	-1.809742	-1.273290	-1.626162

H	-2.187153	0.230776	2.013662
H	-2.926818	-2.287451	0.807659
H	-0.784413	-0.858824	2.139546
H	0.891649	2.062859	0.776612
H	0.611289	-1.936018	-0.782068
H	3.354847	1.933257	0.674798
H	3.077486	-2.066915	-0.889818
H	4.468934	-0.133470	-0.160105

4b-TSII

C	-1.664654	-1.392432	-0.558656
C	-0.865260	-0.103532	-0.382748
C	-1.604855	1.126293	-0.982175
C	-2.256531	1.479458	0.333265
C	-2.137684	0.250993	1.053569
C	-2.762540	-1.042148	0.468580
C	0.595736	-0.069426	-0.198024
C	1.365813	-1.249777	-0.096017
C	2.744757	-1.204623	0.108945
C	3.404756	0.021480	0.232584
C	2.661875	1.203123	0.143623
C	1.285547	1.159428	-0.071394
H	-2.873700	-1.811925	1.239402
H	-3.754894	-0.858877	0.038107
H	-2.011226	-1.554630	-1.589309
H	-1.112818	-2.283455	-0.250832
H	-2.012637	0.274439	2.140103
H	-2.283179	0.833210	-1.797463
H	-2.171171	2.457700	0.799948
H	-0.948641	1.907139	-1.381283
H	0.887985	-2.219364	-0.190731
H	0.736588	2.094483	-0.123471
H	3.305868	-2.134184	0.170120
H	3.157281	2.166365	0.240854
H	4.478785	0.056086	0.395243

4c

C	0.611747	-0.908899	1.181341
C	0.024322	0.091030	0.124596
C	0.496982	1.575177	0.320459

C	1.690184	1.235526	-0.534347
C	1.266243	-0.176746	-0.802419
C	1.795260	-1.235937	0.224598
C	-1.402123	-0.152518	-0.293018
O	-1.681683	-0.694012	-1.351582
C	-2.480506	0.296961	0.679955
H	1.749389	-2.256157	-0.170672
H	2.801196	-1.055184	0.616528
H	0.880380	-0.443848	2.136472
H	-0.036604	-1.767372	1.386720
H	1.165939	-0.512053	-1.839941
H	0.678347	1.888561	1.360601
H	2.615642	1.770780	-0.730828
H	-0.182634	2.317948	-0.130175
H	-2.271977	-0.068382	1.693335
H	-2.501510	1.393256	0.735050
H	-3.457353	-0.063015	0.348587

4c-TSI

C	-1.148087	-0.629512	-0.771319
C	-1.480017	-1.507879	0.243916
C	-0.552784	-0.877731	1.260414
C	-0.061665	0.064471	0.079370
C	-0.584760	1.518866	0.137740
C	-1.990400	1.263852	-0.377347
C	1.399176	-0.108504	-0.279312
C	2.409685	0.533305	0.658005
O	1.750181	-0.715024	-1.278780
H	-2.297800	1.706741	-1.322261
H	-2.794628	1.108283	0.337111
H	-0.532759	1.979291	1.133091
H	-0.027112	2.161758	-0.554944
H	-1.256697	-0.704316	-1.849211
H	-1.020985	-0.340723	2.099528
H	-2.207908	-2.309494	0.330932
H	0.221585	-1.540342	1.672429
H	2.341008	1.626996	0.587111
H	2.206177	0.268497	1.702735
H	3.420783	0.222286	0.384919

4c-TSII

C	1.256404	0.330177	-0.974576
C	1.205679	1.589287	-0.295313
C	0.481720	1.233028	0.979518
C	-0.014887	-0.116550	0.404194
C	0.901429	-1.299106	0.681193
C	1.980630	-0.891060	-0.342390
C	-1.414192	-0.338909	-0.015758
C	-2.314287	0.870003	-0.216403
O	-1.834292	-1.476349	-0.240527
H	2.156996	-1.666125	-1.094801
H	2.951751	-0.608992	0.081699
H	1.237145	-1.355334	1.724485
H	0.409344	-2.238126	0.419046
H	1.171309	0.315423	-2.065532
H	1.095932	1.095222	1.880843
H	1.102401	2.543711	-0.805839
H	-0.311682	1.944922	1.234855
H	-2.605016	1.295450	0.753633
H	-1.811165	1.664516	-0.781236
H	-3.217651	0.558907	-0.745716

4d

C	-2.397124	-0.877820	0.176641
C	-3.640594	0.052228	-0.002813
C	-2.832228	0.860639	-0.986150
C	-1.599634	0.030786	-0.833557
C	-0.635327	0.482086	0.354933
C	-1.417261	-0.485825	1.308206
H	-0.779506	1.537377	0.608427
H	-1.866233	-0.016946	2.192159
H	-0.797351	-1.322930	1.645889
H	-1.081506	-0.338070	-1.726198
H	-3.984593	0.564793	0.910440
H	-3.014879	1.814725	-1.476181
H	-4.518861	-0.452661	-0.436266
H	-2.563793	-1.945375	0.006430
C	0.837628	0.226844	0.159639
C	1.765733	1.269445	0.306367
C	1.326390	-1.044753	-0.189641
C	3.134262	1.054515	0.117689
H	1.410392	2.262592	0.574028

C	2.691555	-1.264414	-0.382175
H	0.633939	-1.874660	-0.314923
C	3.603205	-0.214720	-0.228298
H	3.831736	1.879611	0.241225
H	3.044653	-2.256658	-0.653088
H	4.666363	-0.385866	-0.376977

4d-TSI

C	-2.504361	-0.833846	-0.153029
C	-3.552172	0.303468	0.143010
C	-2.756002	1.177591	-0.801538
C	-1.729823	0.235467	-0.967512
C	-0.578705	0.110842	0.656567
C	-1.459996	-1.111553	0.932900
H	-0.850732	1.001790	1.220984
H	-1.843221	-1.164003	1.960930
H	-0.927276	-2.048278	0.737374
H	-1.017347	0.124115	-1.783377
H	-3.589620	0.625302	1.195982
H	-2.885664	2.205683	-1.130538
H	-4.580826	0.074270	-0.169745
H	-2.927323	-1.703164	-0.668649
C	0.848346	0.042179	0.348710
C	1.655279	1.190679	0.529399
C	1.469413	-1.108830	-0.188421
C	3.008898	1.187532	0.202520
H	1.202629	2.091562	0.938963
C	2.825329	-1.110783	-0.515018
H	0.888147	-2.011723	-0.353539
C	3.605415	0.034504	-0.322438
H	3.603139	2.084474	0.360575
H	3.276343	-2.012436	-0.922930
H	4.662019	0.028908	-0.576937

4d-TSII

C	-2.552640	0.822463	-0.537177
C	-3.547965	-0.261367	-0.081617
C	-2.810070	-0.537756	1.207728
C	-1.524385	0.015104	0.981272
C	-0.665316	-0.461506	-0.241973

C	-1.370798	0.355639	-1.355501
H	-0.820803	-1.539000	-0.377140
H	-1.626920	-0.223849	-2.256607
H	-0.749043	1.200844	-1.669116
H	-0.947199	0.396823	1.828851
H	-3.623069	-1.094134	-0.798437
H	-3.293025	-0.529264	2.181637
H	-2.908414	1.851200	-0.607185
H	-4.564607	0.114489	0.087774
C	0.821897	-0.220854	-0.093858
C	1.733352	-1.275901	-0.244311
C	1.330855	1.057173	0.194412
C	3.110378	-1.065672	-0.120266
H	1.360032	-2.274643	-0.461502
C	2.704243	1.272048	0.323351
H	0.646674	1.893615	0.322048
C	3.601078	0.210238	0.164662
H	3.796669	-1.899948	-0.244045
H	3.075321	2.268967	0.549049
H	4.670611	0.377247	0.264335

4e

C	2.775126	0.398981	-0.194727
C	2.927848	-0.357907	1.157957
C	1.869714	-1.316049	0.674440
C	1.769505	-0.709027	-0.695178
C	0.680810	0.407128	-0.911969
C	1.622282	1.441980	-0.218553
H	0.646309	0.627205	-1.988970
H	1.297963	1.744856	0.783708
H	1.817560	2.346309	-0.803814
H	1.958901	-1.362340	-1.557024
H	2.716017	0.225572	2.067700
H	1.286192	-2.078709	1.183186
H	3.920873	-0.819237	1.291682
H	3.685962	0.656937	-0.741539
C	-0.730422	0.194873	-0.417497
C	-1.350054	-1.058406	-0.548715
C	-1.473511	1.244818	0.141776
C	-2.668869	-1.257212	-0.134387
H	-0.792195	-1.888299	-0.977492
C	-2.794539	1.051276	0.557505

H	-1.017465	2.225801	0.253268
C	-3.397770	-0.201456	0.422052
H	-3.126615	-2.237694	-0.243245
H	-3.350704	1.880472	0.988542
H	-4.423521	-0.354869	0.747772

4e-TSI

C	2.715094	-0.165819	-0.341356
C	2.582694	1.276385	0.271255
C	1.934372	0.625495	1.472153
C	1.973249	-0.666485	0.928611
C	0.593144	-1.066233	-0.455885
C	1.672481	-0.537063	-1.408436
H	0.588744	-2.153081	-0.366682
H	1.355817	0.305516	-2.033913
H	2.018019	-1.326868	-2.087305
H	2.027408	-1.616911	1.457529
H	1.970023	1.979581	-0.313263
H	1.521495	1.035845	2.389817
H	3.545663	1.768717	0.473362
H	3.744948	-0.487693	-0.530319
C	-0.733662	-0.479637	-0.283258
C	-1.765263	-1.250745	0.301080
C	-1.037208	0.855319	-0.628105
C	-3.032536	-0.719173	0.525490
H	-1.559391	-2.283614	0.575880
C	-2.307875	1.387225	-0.406061
H	-0.274659	1.482678	-1.079844
C	-3.313701	0.606573	0.172277
H	-3.806035	-1.339778	0.971789
H	-2.513840	2.417486	-0.687052
H	-4.302925	1.023068	0.343416

4e-TSII

C	2.807761	-0.584423	-0.414463
C	3.021467	0.929885	-0.358231
C	2.195202	1.099116	0.890030
C	1.619657	-0.182640	1.135077
C	0.634439	-0.928893	0.190082
C	1.515705	-1.014418	-1.083499

H	0.563111	-1.946055	0.593440
H	1.205789	-0.319180	-1.874376
H	1.536435	-2.021105	-1.513769
H	1.480592	-0.465180	2.186617
H	2.693166	1.450077	-1.271783
H	2.429036	1.807713	1.682157
H	4.069142	1.213953	-0.183310
H	3.666861	-1.253329	-0.375331
C	-0.775559	-0.377536	0.084399
C	-1.018183	0.965497	-0.246598
C	-1.879841	-1.215333	0.302022
C	-2.321756	1.451781	-0.362178
H	-0.177922	1.637670	-0.400427
C	-3.187767	-0.733629	0.188926
H	-1.713596	-2.258881	0.563749
C	-3.412912	0.603504	-0.145516
H	-2.486915	2.495880	-0.617525
H	-4.027209	-1.402389	0.363851
H	-4.427769	0.983360	-0.233591

4f

C	-1.495888	-0.751021	-0.445952
C	-2.692798	0.090231	0.103612
C	-1.843003	1.323639	-0.067476
C	-0.660565	0.576676	-0.588103
C	0.333552	0.025322	0.543137
C	-0.502121	-1.279570	0.616409
H	0.328114	0.654249	1.440184
H	-0.933417	-1.509747	1.597123
H	0.079633	-2.138369	0.270093
H	-0.176056	0.907674	-1.514473
H	-3.020703	-0.160328	1.125243
H	-1.982851	2.361623	0.226169
H	-3.588755	0.063701	-0.537031
H	-1.705829	-1.400240	-1.299474
C	1.752826	-0.109120	0.025507
C	2.634147	1.120378	0.161832
H	2.095840	2.029057	-0.135036
H	2.919533	1.247966	1.214976
H	3.538521	1.006978	-0.440484
O	2.161135	-1.130222	-0.505136

4f-TSI

C	-0.006135	-0.117597	-0.041813
C	0.194488	-0.233672	1.515531
C	1.638804	0.149536	1.285221
C	1.522244	0.146746	-0.111606
C	1.425248	-1.733473	-0.795224
C	-0.069446	-1.430241	-0.826139
H	1.803617	-2.350281	0.018476
H	-0.702639	-2.213119	-0.390682
H	-0.382365	-1.260239	-1.861168
H	2.114703	0.666846	-0.861501
H	0.012451	-1.235213	1.934312
H	2.476465	0.294995	1.962928
H	-0.391475	0.484882	2.105675
H	-0.694892	0.676989	-0.346522
C	2.211740	-1.780355	-2.036502
C	3.629204	-2.325140	-1.938004
H	4.145044	-1.945383	-1.047292
H	3.601558	-3.420088	-1.854021
H	4.193247	-2.058039	-2.834970
O	1.765027	-1.363641	-3.108142

4f-TSII

C	0.035030	-0.042367	0.096349
C	0.083101	-0.197298	1.627447
C	1.555986	0.125540	1.721342
C	2.027640	-0.041700	0.397873
C	1.814275	-1.404439	-0.357886
C	0.328411	-1.277838	-0.721838
H	2.038695	-2.229818	0.332496
H	-0.283505	-2.155386	-0.463126
H	0.225638	-1.088842	-1.794386
H	2.878419	0.556907	0.056957
H	-0.228060	-1.199834	1.959579
H	1.962151	0.869073	2.402455
H	-0.537113	0.530308	2.165572
H	-0.537137	0.785070	-0.323270
C	2.771238	-1.526895	-1.543244
C	4.211072	-1.873757	-1.207300
H	4.546996	-1.380283	-0.288084

H	4.280705	-2.956671	-1.034071
H	4.867944	-1.611708	-2.040319
O	2.411242	-1.353481	-2.694760

4g

C	1.822662	0.423851	-0.429620
C	2.157718	-0.479270	0.798218
C	1.067187	-1.412980	0.341734
C	0.725086	-0.615640	-0.878162
C	-0.370393	0.531763	-0.708417
C	0.724736	1.493579	-0.180309
H	-0.743189	0.816974	-1.700752
H	0.591685	1.776874	0.868071
H	0.833180	2.404087	-0.777934
H	0.707574	-1.124636	-1.849600
H	2.035163	-0.007536	1.785115
H	0.610143	-2.285921	0.801553
H	3.169501	-0.915727	0.768074
H	2.652421	0.705270	-1.083044
C	-1.547689	0.197347	0.183177
C	-2.599466	-0.726419	-0.407754
H	-3.158423	-0.196454	-1.190944
H	-2.135503	-1.600630	-0.881300
H	-3.295568	-1.049970	0.369628
O	-1.643255	0.625535	1.322241

4g-TSI

C	1.759401	0.580016	-0.178239
C	1.905758	-0.656706	0.783240
C	1.221145	-1.475858	-0.284250
C	0.985055	-0.379086	-1.126084
C	-0.496476	0.826007	-0.523374
C	0.641173	1.574304	0.168226
H	-0.839484	1.224276	-1.478492
H	0.474128	1.707212	1.241869
H	0.800161	2.560551	-0.283269
H	0.854205	-0.368787	-2.207034
H	1.369724	-0.567308	1.737000
H	0.945471	-2.526095	-0.335635
H	2.945905	-0.944528	0.994797

H	2.709920	1.004942	-0.517982
C	-1.506696	0.086602	0.244367
C	-2.713205	-0.440265	-0.518820
H	-3.391101	0.387662	-0.766822
H	-2.414493	-0.908957	-1.464825
H	-3.253336	-1.163737	0.096594
O	-1.372253	-0.136915	1.449176

4g-TSII

C	-1.905375	-0.552850	-0.336694
C	-2.019228	0.281744	0.947160
C	-1.191528	1.419355	0.404305
C	-0.597945	0.900170	-0.776544
C	0.318331	-0.370195	-0.775762
C	-0.701502	-1.466983	-0.419759
H	0.678633	-0.507624	-1.804840
H	-0.471256	-1.983430	0.519924
H	-0.788274	-2.219446	-1.209620
H	-0.384909	1.599239	-1.592831
H	-1.631333	-0.244558	1.831738
H	-1.442287	2.469480	0.534514
H	-3.046325	0.595862	1.176514
H	-2.804885	-0.751162	-0.918479
C	1.556622	-0.238978	0.109071
C	2.445498	0.969814	-0.125002
H	2.553465	1.195041	-1.192725
H	1.988494	1.848366	0.348498
H	3.426520	0.799220	0.325106
O	1.811615	-1.056682	0.977693

5a

C	-1.732371	-0.440597	0.539839
C	-1.576208	0.353826	-0.772153
C	-0.079023	0.676437	-0.859084
C	0.674525	-0.465749	0.004409
C	-0.476342	-1.331473	0.572402
C	0.450255	1.753019	0.126566
C	1.167535	0.665723	0.968593
C	1.734342	-1.243130	-0.664947

H	-1.869568	-0.277440	-1.622580
H	-2.200691	1.256682	-0.805439
H	0.274441	0.792562	-1.887955
H	-0.241909	-1.713580	1.573823
H	-0.627170	-2.202143	-0.081251
H	-2.663664	-1.017296	0.582662
H	-1.738676	0.242848	1.399950
H	-0.335635	2.306424	0.654927
H	1.124635	2.483830	-0.332339
H	2.258007	0.764354	1.002331
H	0.805927	0.560298	1.998514
H	2.735552	-0.837142	-0.787497
H	1.502470	-2.167735	-1.188898

5a-TSI

C	-0.635129	-1.323277	0.582018
C	-1.760626	-0.268436	0.548753
C	-1.512554	0.492367	-0.770920
C	0.021521	0.604393	-0.879148
C	0.539625	-0.683189	-0.172770
C	0.656505	1.689795	0.023264
C	1.215147	0.816896	1.134833
C	1.611446	-1.424691	-0.625541
H	-1.895186	-0.100959	-1.613008
H	-2.010271	1.469246	-0.805915
H	0.348008	0.677295	-1.923119
H	-0.366515	-1.635700	1.597253
H	-0.955137	-2.224920	0.041360
H	-2.759652	-0.715911	0.598140
H	-1.674403	0.416608	1.402612
H	-0.068906	2.435313	0.376433
H	1.452157	2.234606	-0.498536
H	2.291551	0.727479	1.255901
H	0.647064	0.704151	2.056842
H	1.848335	-2.396190	-0.196747
H	2.327344	-1.014166	-1.334149

5a-TSII

C	-1.931802	-0.945810	0.731558
C	-0.881578	-0.463727	-0.041522

C	-1.089863	0.789901	-0.919784
C	-0.129942	1.778176	-0.215494
C	0.378432	0.859150	0.891097
C	1.687946	0.141075	0.704078
C	1.574837	-0.731360	-0.561750
C	0.209568	-1.434904	-0.490223
H	1.891476	-0.491928	1.578374
H	2.532133	0.846718	0.616878
H	0.069921	1.078782	1.911971
H	-0.058724	-1.866338	-1.465713
H	0.257912	-2.267197	0.224670
H	2.399814	-1.449826	-0.641492
H	1.624062	-0.096048	-1.456450
H	0.676163	2.146455	-0.865107
H	-0.651365	2.655713	0.182959
H	-2.133468	1.122032	-0.888128
H	-0.839470	0.599329	-1.972357
H	-2.829814	-0.355881	0.899593
H	-1.844220	-1.876815	1.287045

5b

C	2.565551	-0.172243	1.514894
C	1.084132	0.214960	1.655606
C	0.557103	0.446564	0.217166
C	1.597897	-0.420698	-0.732595
C	2.581889	-1.067426	0.264939
C	1.114305	1.750006	-0.428520
C	2.103305	0.945524	-1.302544
C	1.068302	-1.357004	-1.737237
H	0.530935	-0.613816	2.115301
H	0.922967	1.100023	2.285263
H	3.582035	-1.180210	-0.172574
H	2.225793	-2.074189	0.527303
H	2.954003	-0.679077	2.405789
H	3.187193	0.719353	1.357809
H	1.574432	2.443329	0.285326
H	0.381114	2.308509	-1.016190
H	1.933963	1.051463	-2.378995
H	3.165079	1.136162	-1.107082
H	0.568022	-0.993969	-2.631065
H	1.049969	-2.429215	-1.558887
C	-0.932139	0.195498	0.114494

C	-1.440118	-1.113660	0.199737
C	-1.857059	1.244513	0.000278
C	-2.811853	-1.365835	0.157229
H	-0.750903	-1.947954	0.299678
C	-3.234193	0.998689	-0.036637
H	-1.507157	2.271732	-0.051855
C	-3.718877	-0.307964	0.036837
H	-3.173063	-2.389865	0.217582
H	-3.925767	1.833621	-0.122499
H	-4.788082	-0.501445	0.003214

5b-TSI

C	2.547179	-1.166458	0.357276
C	2.505518	-0.220745	1.571978
C	1.036307	0.235010	1.623081
C	0.563571	0.384951	0.142448
C	1.505029	-0.620390	-0.623775
C	1.063777	1.709243	-0.502021
C	2.330076	1.240071	-1.190398
C	1.162660	-1.293247	-1.775579
H	0.433548	-0.543618	2.107168
H	0.882816	1.160428	2.190859
H	3.541440	-1.253243	-0.094671
H	2.244814	-2.177450	0.668155
H	2.816861	-0.714970	2.499206
H	3.175733	0.634725	1.425975
H	1.225621	2.514853	0.227359
H	0.347590	2.077579	-1.243905
H	2.390674	1.284463	-2.274238
H	3.286231	1.334204	-0.680768
H	1.819897	-2.052866	-2.193394
H	0.293353	-1.015686	-2.365684
C	-0.940875	0.152003	0.052580
C	-1.480887	-1.145723	0.064390
C	-1.838866	1.231105	0.048624
C	-2.861021	-1.356594	0.055946
H	-0.812633	-2.002311	0.066574
C	-3.222497	1.025614	0.044271
H	-1.461171	2.250028	0.055268
C	-3.741255	-0.270298	0.044327
H	-3.248686	-2.372705	0.056299
H	-3.892313	1.882384	0.040905

H	-4.816075	-0.433068	0.036008

5b-TSII

C	-1.075329	-0.500616	2.174975
C	-1.686314	-0.064244	0.985543
C	-2.009263	1.435859	0.812769
C	-1.119235	1.726434	-0.414659
C	-0.493314	0.324254	-0.532543
C	-1.145043	-0.557371	-1.592245
C	-2.623922	-0.762466	-1.227086
C	-2.643151	-1.030511	0.285049
H	-0.638279	-1.527745	-1.641929
H	-1.035181	-0.093798	-2.585878
H	-3.656269	-0.925284	0.698678
H	-2.321345	-2.061627	0.485490
H	-3.076624	-1.581790	-1.798116
H	-3.203657	0.140598	-1.459225
H	-1.678820	2.008657	-1.315529
H	-0.396883	2.523486	-0.224507
H	-1.704227	2.009495	1.694592
H	-3.079968	1.620693	0.654073
H	-0.572664	0.195489	2.841662
H	-0.957741	-1.559438	2.392964
C	0.962233	0.130044	-0.303417
C	1.477158	-1.165331	-0.074740
C	1.883216	1.195594	-0.290336
C	2.835246	-1.383404	0.146519
H	0.798234	-2.013379	-0.051431
C	3.247554	0.979140	-0.076720
H	1.543694	2.210677	-0.469145
C	3.733727	-0.310461	0.144046
H	3.194156	-2.394069	0.326922
H	3.930334	1.825615	-0.086335
H	4.793864	-0.479109	0.314787

5c

C	1.915191	1.313261	-0.441031
C	0.429123	1.463359	-0.820152
C	-0.210050	0.097734	-0.511396
C	0.763047	-0.565714	0.671742

C	1.874509	0.489994	0.855793
C	0.227415	-1.044576	-1.460229
C	1.105509	-1.687560	-0.361416
C	0.162620	-1.024707	1.933347
H	-0.020646	2.253281	-0.206839
H	0.283275	1.743063	-1.871833
H	2.834806	0.016657	1.095969
H	1.614780	1.143855	1.700332
H	2.416650	2.279583	-0.315333
H	2.457285	0.769098	-1.225087
H	0.774169	-0.694775	-2.342845
H	-0.611981	-1.661580	-1.787783
H	0.760479	-2.676092	-0.042027
H	2.175525	-1.758142	-0.589985
H	-0.412287	-1.945793	1.975695
H	0.187144	-0.407051	2.827814
C	-1.688643	0.120603	-0.170192
C	-2.207290	1.218941	0.746267
H	-1.489267	1.481310	1.530087
H	-2.403110	2.126331	0.159427
H	-3.147955	0.892773	1.196185
O	-2.455933	-0.731316	-0.595021

5c-TSI

C	-1.831276	-0.853069	0.730644
C	-1.855131	-1.226473	-0.762810
C	-0.373462	-1.147224	-1.181690
C	0.197278	0.087416	-0.430857
C	-0.671916	0.138715	0.883202
C	-0.214346	1.430164	-1.076161
C	-1.347039	1.847312	-0.157900
C	-0.193010	0.528440	2.115330
H	0.136590	-2.062298	-0.857458
H	-0.231677	-1.059601	-2.264977
H	-2.780424	-0.439977	1.089062
H	-1.620149	-1.747129	1.334664
H	-2.284491	-2.217832	-0.944668
H	-2.453030	-0.506838	-1.334944
H	-0.518660	1.319088	-2.124899
H	0.620577	2.135763	-1.047303
H	-1.218485	2.712511	0.486820
H	-2.376861	1.647825	-0.448154

H	-0.800929	0.412991	3.009779
H	0.733265	1.087885	2.222312
C	1.701847	-0.036257	-0.162166
C	2.225208	-1.308718	0.490445
H	1.481881	-1.804500	1.120112
H	2.534173	-2.010986	-0.295402
H	3.110278	-1.063791	1.083441
O	2.479877	0.854382	-0.464576

5c-TSII

C	0.298492	-1.316107	1.782559
C	0.881855	-0.716447	0.641219
C	1.104303	-1.583106	-0.621228
C	0.212298	-0.780210	-1.590817
C	-0.293850	0.240074	-0.562472
C	0.374370	1.604024	-0.585985
C	1.868901	1.395963	-0.277341
C	1.907475	0.393383	0.885355
H	-0.063075	2.266737	0.169065
H	0.231711	2.089646	-1.563804
H	2.907704	-0.044865	1.008131
H	1.663798	0.904979	1.826320
H	2.372607	2.337132	-0.027774
H	2.384547	0.983421	-1.154037
H	0.759219	-0.306865	-2.414813
H	-0.608354	-1.367754	-2.008150
H	0.746268	-2.606115	-0.468569
H	2.163235	-1.637369	-0.905179
H	-0.250825	-2.250529	1.709010
H	0.269511	-0.796958	2.737901
C	-1.714873	0.109660	-0.140111
C	-2.309750	1.152163	0.795369
H	-1.659298	1.338337	1.658632
H	-2.444966	2.109798	0.276139
H	-3.283331	0.799149	1.142418
O	-2.395510	-0.851890	-0.493073

5d

C	-3.276518	0.933841	-0.500960
C	-3.440478	-0.591241	-0.348386

C	-2.038540	-1.105669	0.007774
C	-1.255123	0.132437	0.671396
C	-2.277479	1.299726	0.612201
C	-0.997420	-1.134991	-1.139655
C	-0.267926	0.120092	-0.579342
C	-0.673565	-0.062406	2.012560
H	-4.133316	-0.806536	0.476848
H	-3.847128	-1.072572	-1.247667
H	-2.064482	-2.017715	0.611860
H	-1.781062	2.265443	0.454581
H	-2.806004	1.360339	1.573784
H	-4.224803	1.476725	-0.413661
H	-2.860077	1.175711	-1.488213
H	-1.409799	-1.007318	-2.148079
H	-0.381872	-2.039505	-1.144633
H	-0.474948	1.000944	-1.198112
H	0.357218	-0.362866	2.164078
H	-1.314590	0.002359	2.888862
C	1.224728	0.067310	-0.352304
C	1.997723	1.225106	-0.541723
C	1.888653	-1.099167	0.063665
C	3.377607	1.224178	-0.323542
H	1.509004	2.140457	-0.870083
C	3.268622	-1.107252	0.283249
H	1.326377	-2.015829	0.222601
C	4.020565	0.055011	0.091224
H	3.949684	2.135186	-0.482572
H	3.756139	-2.024808	0.604283
H	5.094555	0.048136	0.259180

5d-TSI

C	-3.218782	1.011896	-0.531632
C	-3.436304	-0.513490	-0.440998
C	-2.080705	-1.087081	0.016906
C	-2.285041	1.326113	0.656875
C	-0.994351	-1.196046	-1.075301
C	-0.179994	0.043227	-0.706416
C	-0.782544	-0.174750	2.065542
H	-4.196522	-0.729709	0.322026
H	-3.785024	-0.954787	-1.382836
H	-2.209545	-2.016503	0.583434
H	-1.676139	2.224598	0.500336

H	-2.882556	1.497781	1.562771
H	-4.157678	1.575179	-0.488035
H	-2.737767	1.270751	-1.484144
H	-1.377317	-1.166807	-2.105095
H	-0.411491	-2.117443	-0.977948
H	-0.498005	0.954205	-1.213334
H	-0.388371	-1.155678	2.318979
H	-0.500991	0.647372	2.719784
C	1.258802	0.030564	-0.437069
C	1.999352	1.227660	-0.559765
C	1.952663	-1.120344	-0.005998
C	3.362852	1.273004	-0.276364
H	1.489610	2.130323	-0.891378
C	3.318527	-1.076857	0.275001
H	1.421303	-2.060427	0.112743
C	4.033332	0.117928	0.142281
H	3.905865	2.208683	-0.387056
H	3.827588	-1.980782	0.601458
H	5.097523	0.148686	0.361293
C	-1.434557	0.058935	0.851440

5d-TSII

C	3.293138	-0.773031	-0.594311
C	3.449593	0.725622	-0.271549
C	2.083206	1.278123	0.030071
C	2.343493	-1.354388	0.465508
C	0.984628	1.171665	-1.018269
C	0.274890	-0.128353	-0.545512
C	0.638993	-0.353574	2.005447
H	4.103049	0.855398	0.601689
H	3.930472	1.256432	-1.111393
H	2.020246	2.097992	0.743824
H	1.978711	-2.346615	0.161474
H	2.885176	-1.490418	1.410799
H	4.257343	-1.295822	-0.603488
H	2.862512	-0.893727	-1.597629
H	1.373610	1.089107	-2.042728
H	0.317124	2.038603	-1.002149
H	0.449574	-0.939330	-1.264865
H	-0.327438	0.089376	2.222025
H	1.243797	-0.656026	2.857077
C	-1.225143	-0.049106	-0.331914

C	-2.035726	-1.136531	-0.695068
C	-1.852128	1.073678	0.233075
C	-3.419055	-1.110451	-0.501045
H	-1.574741	-2.017165	-1.138318
C	-3.235110	1.106146	0.430796
H	-1.259669	1.936144	0.527955
C	-4.025943	0.013771	0.064435
H	-4.021398	-1.966468	-0.795826
H	-3.694381	1.988064	0.871134
H	-5.102272	0.040398	0.214570
C	1.151543	-0.427895	0.719314

5e

C	1.886189	-0.949502	1.571081
C	2.980062	-1.063441	0.490769
C	2.401680	-0.312732	-0.711787
C	1.432170	0.825814	-0.115319
C	1.334207	0.479583	1.394580
C	1.187493	-0.979211	-1.410414
C	0.293964	0.236912	-1.056096
C	1.775766	2.238686	-0.367043
H	3.898645	-0.566706	0.833115
H	3.239648	-2.103005	0.249392
H	3.161829	0.059019	-1.405010
H	0.315079	0.591715	1.779495
H	1.966575	1.184447	1.950740
H	2.268637	-1.127379	2.582882
H	1.095164	-1.689599	1.395710
H	0.890960	-1.912240	-0.920349
H	1.300071	-1.182705	-2.480456
H	0.231559	0.897770	-1.930622
H	1.655376	2.672517	-1.357310
H	2.283285	2.840773	0.382566
C	-1.105874	0.060772	-0.511853
C	-1.810834	1.185909	-0.045895
C	-1.754859	-1.181150	-0.476540
C	-3.112025	1.072054	0.444151
H	-1.327671	2.160866	-0.067686
C	-3.061906	-1.300013	0.010625
H	-1.245998	-2.069145	-0.841115
C	-3.745344	-0.175624	0.475458
H	-3.633913	1.957323	0.800030

H	-3.543482	-2.275026	0.023185
H	-4.759892	-0.266966	0.855130

5e-TSI

C	-2.056401	-1.542740	-0.921890
C	-3.070547	-1.024297	0.123069
C	-2.375209	0.191846	0.754422
C	-1.574543	0.825163	-0.417168
C	-1.351369	-0.275173	-1.470588
C	-1.183018	-0.125208	1.687033
C	-0.140794	0.727405	0.970167
C	-1.755544	2.149227	-0.834155
H	-3.992339	-0.697704	-0.377206
H	-3.348215	-1.786753	0.862019
H	-3.082354	0.894306	1.209283
H	-0.288775	-0.453682	-1.671130
H	-1.805626	0.039716	-2.417780
H	-2.537399	-2.126314	-1.714745
H	-1.326979	-2.207359	-0.443073
H	-0.934564	-1.191320	1.680398
H	-1.332230	0.162207	2.735831
H	-0.141962	1.766313	1.294900
H	-2.138542	2.908421	-0.155595
H	-1.384459	2.492429	-1.797335
C	1.174989	0.274395	0.531034
C	2.138857	1.235359	0.139047
C	1.540212	-1.087289	0.428796
C	3.395436	0.857650	-0.325140
H	1.884385	2.291034	0.207524
C	2.802850	-1.464540	-0.029966
H	0.836774	-1.860198	0.723622
C	3.738247	-0.497920	-0.412228
H	4.114476	1.620421	-0.614648
H	3.057793	-2.520201	-0.087493
H	4.721017	-0.794586	-0.769164

5e-TSII

C	1.952337	-0.543175	1.690954
C	3.018615	-0.992060	0.672444
C	2.486446	-0.700520	-0.702809

C	1.317472	0.946587	-0.281696
C	1.445888	0.839453	1.241176
C	1.137266	-1.274525	-1.107724
C	0.303311	0.029087	-1.027352
C	1.698589	2.139731	-0.882274
H	3.954237	-0.439702	0.833375
H	3.253412	-2.062682	0.803275
H	3.199459	-0.473949	-1.493424
H	0.484183	1.068323	1.718241
H	2.152387	1.612192	1.570638
H	2.352734	-0.508764	2.711594
H	1.122619	-1.260835	1.706565
H	0.801191	-2.038398	-0.396699
H	1.131500	-1.731897	-2.103855
H	0.226643	0.435435	-2.045239
H	1.473064	2.348588	-1.925622
H	2.332057	2.856467	-0.364806
C	-1.109294	-0.032741	-0.464497
C	-1.752928	1.144598	-0.045218
C	-1.829765	-1.234530	-0.401300
C	-3.065642	1.119565	0.428701
H	-1.215550	2.088972	-0.092956
C	-3.146619	-1.263865	0.070867
H	-1.367929	-2.161129	-0.731435
C	-3.769854	-0.087460	0.490840
H	-3.539800	2.044210	0.749593
H	-3.683064	-2.209133	0.107887
H	-4.792083	-0.108572	0.860198

5f

C	2.428884	-0.496493	-0.920138
C	2.588031	0.678449	0.065968
C	1.181601	0.921267	0.631829
C	0.397958	-0.477646	0.469936
C	1.411115	-1.417493	-0.222036
C	0.160753	1.606740	-0.309380
C	-0.564721	0.269401	-0.568194
C	-0.225974	-1.043146	1.681568
H	3.267812	0.387604	0.878510
H	3.007840	1.577972	-0.402822
H	1.197368	1.325765	1.647840
H	0.921271	-2.120959	-0.907199

H	1.923031	-2.014988	0.545377
H	3.376194	-1.002703	-1.137826
H	2.030947	-0.138974	-1.879717
H	0.589834	2.079624	-1.200539
H	-0.485464	2.328804	0.197127
H	-0.410401	-0.135929	-1.576116
H	-1.085850	-0.570468	2.148183
H	0.274676	-1.830514	2.239054
C	-2.048180	0.209153	-0.251340
C	-2.790349	-1.025760	-0.728295
H	-2.855955	-1.015626	-1.824849
H	-2.248032	-1.936244	-0.445036
H	-3.798864	-1.046710	-0.308618
O	-2.617389	1.095813	0.365890

5f-TSI

C	-2.414754	0.487220	-0.966158
C	-2.568436	-0.724472	-0.023392
C	-1.173613	-0.919071	0.601343
C	-0.574796	0.521150	0.648644
C	-1.479621	1.438402	-0.191139
C	-0.122389	-1.574381	-0.319859
C	0.678046	-0.329400	-0.670593
C	0.105622	1.022215	1.762241
H	-3.293807	-0.485455	0.766407
H	-2.926721	-1.625579	-0.535501
H	-1.228944	-1.391379	1.587716
H	-0.914781	2.116954	-0.840818
H	-2.069710	2.065739	0.490911
H	-3.373143	0.954342	-1.217765
H	-1.952751	0.176093	-1.912328
H	-0.547294	-2.078399	-1.197396
H	0.511100	-2.287539	0.215492
H	0.421172	0.196806	-1.589820
H	0.570481	0.358600	2.486033
H	0.316332	2.085312	1.859266
C	2.087756	-0.208588	-0.261638
C	2.873999	0.963613	-0.827925
H	2.978080	0.867266	-1.916689
H	2.349917	1.909119	-0.635822
H	3.866876	0.999000	-0.373634
O	2.602789	-0.990126	0.538101

5f-TSII

C	2.387355	-0.499947	-0.917762
C	2.631132	0.682783	0.041659
C	1.312336	1.103154	0.631809
C	0.276422	-0.675411	0.453473
C	1.408801	-1.453976	-0.212522
C	0.184484	1.581198	-0.271668
C	-0.543624	0.244464	-0.512504
C	-0.267021	-1.143622	1.641043
H	3.312021	0.375316	0.846441
H	3.122886	1.515588	-0.489640
H	1.321096	1.471505	1.656103
H	0.993514	-2.182140	-0.925015
H	1.938383	-2.029013	0.558542
H	3.321168	-1.007660	-1.187856
H	1.949390	-0.134022	-1.856343
H	0.533489	2.059008	-1.197848
H	-0.477369	2.283203	0.244166
H	-0.412286	-0.128141	-1.538430
H	-1.171716	-0.722483	2.070700
H	0.283545	-1.850904	2.256333
C	-2.044766	0.243746	-0.226816
C	-2.833755	-0.935086	-0.767023
H	-2.945747	-0.823718	-1.854590
H	-2.307730	-1.879201	-0.587064
H	-3.826446	-0.964624	-0.311423
O	-2.587799	1.141683	0.394724

5g

C	-0.703566	0.285909	-1.420265
C	-1.509888	-1.011474	-1.213449
C	-2.399641	-0.702730	0.007310
C	-1.499296	0.117177	0.935724
C	-0.457358	0.897753	-0.013495
C	-0.325141	-0.643321	1.606967
C	0.702300	0.230670	0.860872
C	1.816224	-0.442399	0.085288
O	1.842425	-1.649294	-0.102848
C	-0.465850	2.371409	-0.003982

C	2.896141	0.470283	-0.468135
H	-3.267126	-0.101611	-0.299400
H	-2.783204	-1.607834	0.496039
H	-2.051138	0.768988	1.619196
H	0.222049	0.122782	-1.984580
H	-1.303051	1.001624	-1.998596
H	-2.089298	-1.286037	-2.102349
H	-0.834802	-1.846320	-0.994025
H	-0.260972	-1.697209	1.319636
H	-0.282206	-0.577820	2.698767
H	1.143493	1.003002	1.502634
H	-0.116336	2.925015	0.864363
H	-0.950364	2.937987	-0.795008
H	2.461624	1.374957	-0.910997
H	3.547953	0.798835	0.353191
H	3.500431	-0.061670	-1.207096

5g-TSI

C	-0.797445	0.121038	-1.469742
C	-1.608902	-1.128060	-1.055331
C	-2.404594	-0.681728	0.190688
C	-1.439928	0.249969	0.941708
C	-0.637092	0.960708	-0.188798
C	-0.258781	-0.448895	1.652822
C	0.870017	0.271315	0.932487
C	1.852478	-0.440740	0.108668
O	1.713100	-1.628585	-0.200111
C	-0.509639	2.351924	-0.277510
C	3.042243	0.362303	-0.394751
H	-3.298353	-0.118429	-0.112066
H	-2.738277	-1.524468	0.808485
H	-1.959237	0.961189	1.593370
H	0.156880	-0.146592	-1.934379
H	-1.354716	0.718684	-2.202590
H	-2.259066	-1.485418	-1.861451
H	-0.925226	-1.943970	-0.798947
H	-0.219674	-1.522851	1.446371
H	-0.239693	-0.307913	2.739752
H	1.243661	1.179419	1.402192
H	-0.635082	2.988628	0.595308
H	-0.163550	2.830182	-1.191275
H	2.733840	1.353361	-0.750848

H	3.757833	0.521508	0.423336
H	3.545722	-0.181660	-1.197818

5g-TSII

C	0.718674	0.562267	1.373802
C	1.519533	-0.751713	1.327741
C	2.448895	-0.671653	0.100690
C	1.640640	-0.144937	-1.050993
C	0.289080	1.028918	-0.021284
C	0.365496	-0.867607	-1.464098
C	-0.659017	0.106482	-0.853777
C	-1.798009	-0.501820	-0.035995
O	-1.828462	-1.687682	0.251203
C	0.305112	2.389745	-0.294901
C	-2.897772	0.448162	0.402272
H	3.291582	0.003309	0.302388
H	2.878203	-1.662843	-0.123814
H	2.152640	0.447937	-1.806807
H	-0.158053	0.452841	2.028102
H	1.336012	1.356408	1.812923
H	2.083105	-0.905754	2.255875
H	0.837821	-1.603901	1.226215
H	0.280497	-1.866963	-1.023720
H	0.257644	-0.972688	-2.549375
H	-1.117239	0.732710	-1.630380
H	-0.148947	2.796050	-1.195622
H	0.875761	3.080884	0.320695
H	-2.489566	1.410984	0.729369
H	-3.555051	0.652309	-0.454440
H	-3.492509	-0.006880	1.198222

6a

C	0.453134	0.738923	0.673050
C	-0.763064	1.318699	0.032092
C	-1.674167	0.263492	-0.525582
C	-1.250932	-1.032354	0.216052
C	0.223540	-0.811223	0.588073
C	1.278513	-0.883728	-0.557609
C	1.717683	0.573756	-0.249873
H	-1.849873	-1.145312	1.129392

H	0.527419	-1.373202	1.477400
H	-0.895938	2.382525	-0.150123
H	-2.739288	0.499299	-0.390064
H	-1.534713	0.149424	-1.617258
H	0.819195	-0.993863	-1.547182
H	2.648722	0.622176	0.326708
H	1.796716	1.262447	-1.098291
H	0.671432	1.180690	1.655595
H	-1.402635	-1.935652	-0.388449
H	2.050726	-1.653924	-0.454951

6a-TSI

C	-0.352492	-0.582663	-0.693665
C	-0.039263	0.919539	-0.594725
C	1.238442	1.124285	-0.106340
C	1.888426	-0.165913	0.326124
C	0.748960	-1.218188	0.203880
C	-1.609139	0.695616	0.752375
C	-1.761432	-0.575061	-0.070647
H	1.103635	-2.172648	-0.199735
H	-0.305366	-0.982035	-1.717177
H	1.724884	2.092407	-0.018680
H	2.737056	-0.410761	-0.333295
H	2.304684	-0.122325	1.343594
H	-2.018750	-1.476637	0.503401
H	-2.336318	1.500816	0.658317
H	-1.158503	0.616474	1.739716
H	-0.540061	1.643959	-1.234096
H	0.337393	-1.429272	1.198694
H	-2.529666	-0.445666	-0.842751

6a-TSII

C	0.322926	0.949976	-0.689305
C	0.321055	-1.129221	-0.541336
C	-1.032025	-1.209953	-0.212880
C	-1.533555	-0.088067	0.656534
C	-1.045789	1.202482	-0.089062
C	1.404668	-0.738927	0.490089
C	1.516477	0.779781	0.240579
H	-1.757007	1.436190	-0.891058

H	0.502381	1.349548	-1.686903
H	-1.724123	-1.703178	-0.893425
H	-2.621342	-0.092569	0.784334
H	-1.092675	-0.122950	1.663295
H	1.448971	1.390872	1.153273
H	2.340471	-1.277886	0.302603
H	1.089561	-0.987290	1.510810
H	0.668676	-1.702682	-1.401816
H	-1.031556	2.068267	0.591850
H	2.454095	1.045251	-0.260677

6b

C	1.613123	-0.269699	-1.021309
C	2.714041	-1.039683	-0.379674
C	2.713472	-0.877399	1.110914
C	1.248211	-0.504124	1.439044
C	0.703879	0.221253	0.177705
C	1.268149	1.668966	-0.032976
C	1.941193	1.231104	-1.357547
H	0.665789	-1.418041	1.608236
H	3.539176	-1.476321	-0.937346
H	3.048593	-1.777115	1.644950
H	3.401598	-0.069939	1.426345
H	1.981591	1.963120	0.745383
H	1.399726	1.579275	-2.243944
H	3.002489	1.473585	-1.476315
H	1.131288	-0.806010	-1.848112
H	1.151136	0.117516	2.337983
H	0.522531	2.463476	-0.128100
C	-0.799788	0.071722	0.045004
C	-1.674429	1.012729	0.611930
C	-1.364032	-1.054181	-0.577222
C	-3.060524	0.843023	0.551033
H	-1.270958	1.889450	1.112583
C	-2.748681	-1.227338	-0.644262
H	-0.714460	-1.808866	-1.013695
C	-3.605299	-0.277047	-0.081612
H	-3.713779	1.588487	0.998498
H	-3.157569	-2.105992	-1.137680
H	-4.683039	-0.408591	-0.134946

6b-TSI

C	-3.540444	-0.241555	-0.102738
C	-3.005104	0.888018	0.524294
C	-1.622673	1.080309	0.563343
C	-0.741965	0.152783	-0.019824
C	-1.293822	-0.974557	-0.645713
C	-2.678078	-1.171644	-0.687186
C	0.762075	0.374230	0.066981
C	1.623120	-0.393074	-0.958021
C	2.236911	-1.485422	-0.380506
C	2.027352	-1.522258	1.111538
C	1.355748	-0.157553	1.421633
C	2.593251	1.461082	-0.854506
C	1.245759	1.812953	-0.254920
H	0.585792	-0.230879	2.195708
H	2.824273	-2.225246	-0.918370
H	1.378894	-2.367846	1.392262
H	2.960518	-1.657650	1.677464
H	1.287250	2.487258	0.611723
H	2.856396	1.811961	-1.850351
H	3.440240	1.323653	-0.186054
H	1.403691	-0.337252	-2.022367
H	2.114058	0.545872	1.786093
H	0.595987	2.276466	-1.006045
H	-1.222515	1.964819	1.054306
H	-0.635654	-1.706713	-1.106040
H	-3.664625	1.621864	0.981806
H	-3.080573	-2.053810	-1.179749
H	-4.616510	-0.392371	-0.136638

6b-TSII

C	3.615297	-0.247853	0.238484
C	3.084531	1.008483	-0.063610
C	1.716223	1.166740	-0.289070
C	0.824379	0.071031	-0.235398
C	1.387960	-1.191392	0.077187
C	2.751400	-1.347124	0.311006
C	-0.628649	0.211431	-0.446009
C	-1.714598	0.151131	1.249968
C	-2.429607	-1.017457	0.938860
C	-2.751943	-1.147763	-0.524144

C	-1.371274	-0.885251	-1.212576
C	-2.140214	1.534608	0.708593
C	-1.292979	1.591317	-0.578649
H	-0.795595	-1.815327	-1.211741
H	-2.293670	-1.915812	1.538557
H	-3.160503	-2.126427	-0.796881
H	-3.481369	-0.392410	-0.851153
H	-1.890527	1.668100	-1.496669
H	-1.876406	2.323903	1.420647
H	-3.221353	1.598269	0.536573
H	-1.147761	0.161078	2.181744
H	-1.492988	-0.589676	-2.265826
H	-0.592892	2.429755	-0.584034
H	1.346056	2.157766	-0.528654
H	0.742224	-2.060186	0.164143
H	3.738455	1.875165	-0.127706
H	3.142864	-2.331892	0.555647
H	4.680313	-0.369715	0.417506

6c

C	-0.916089	-0.787366	-0.664664
C	-2.094759	0.111303	-0.816185
C	-1.940864	1.380123	-0.030400
C	-0.409838	1.524232	0.156825
C	0.132082	0.075246	0.117625
C	-0.143126	-0.796257	1.400749
C	-0.967517	-1.792450	0.545408
H	0.004729	2.097500	-0.683239
H	-3.028516	-0.198544	-1.278254
H	-2.385555	2.254191	-0.525459
H	-2.442751	1.308043	0.953165
H	-0.732964	-0.256364	2.150126
H	-0.424543	-2.718474	0.330755
H	-1.965211	-2.044085	0.919340
H	-0.574755	-1.239892	-1.602181
H	-0.140761	2.050345	1.080712
H	0.741513	-1.210563	1.897350
C	1.579507	-0.033140	-0.327665
C	2.591027	0.826746	0.415077
H	2.499647	1.869247	0.082827
H	2.410519	0.818537	1.496393
H	3.603947	0.477993	0.200440

O	1.931521	-0.782320	-1.225324

6c-TSI

C	0.132708	0.060558	-0.126516
C	-0.907928	0.346415	0.974856
C	-1.937917	-0.566201	0.922503
C	-1.881990	-1.391753	-0.335983
C	-0.410093	-1.240391	-0.803717
C	-1.254928	1.954793	-0.331309
C	-0.020748	1.362938	-0.982339
C	1.565532	-0.104416	0.369935
O	1.869360	0.061484	1.540161
C	2.616838	-0.457769	-0.671575
H	0.161447	-2.105601	-0.446063
H	-2.775490	-0.592771	1.614148
H	-2.156036	-2.442343	-0.174651
H	-2.585228	-1.006636	-1.094647
H	-0.133731	1.159779	-2.055284
H	-1.171771	2.881941	0.231170
H	-2.224384	1.786378	-0.793356
H	-0.638619	0.903658	1.865779
H	-0.307105	-1.212813	-1.894503
H	0.844465	2.027205	-0.866347
H	2.502033	-1.505968	-0.976222
H	2.505054	0.151643	-1.576204
H	3.615648	-0.321382	-0.250245

6c-TSII

C	0.233412	0.089626	-0.462696
C	-0.921542	0.419971	1.146004
C	-1.671606	-0.762843	1.019700
C	-1.922599	-1.182924	-0.402324
C	-0.492600	-1.123264	-1.034332
C	-1.233602	1.689719	0.317444
C	-0.304833	1.455578	-0.889732
C	1.641328	0.011675	-0.022451
O	2.342478	1.025356	0.054534
C	2.216786	-1.336351	0.393358
H	0.038004	-2.047976	-0.787372
H	-1.646610	-1.513980	1.807080

H	-2.367904	-2.178942	-0.490540
H	-2.590660	-0.480859	-0.921670
H	-0.827651	1.413703	-1.853395
H	-0.975618	2.589635	0.884310
H	-2.297565	1.753388	0.060835
H	-0.409653	0.588405	2.094205
H	-0.539211	-1.058846	-2.131132
H	0.501226	2.189230	-0.960330
H	1.527794	-1.899060	1.034577
H	2.423781	-1.957510	-0.487964
H	3.155789	-1.167150	0.925301

6d

C	-1.302285	0.668487	0.397996
C	-2.385480	1.417579	-0.296992
C	-3.576917	0.542624	-0.556470
C	-3.467507	-0.564575	0.524457
C	-1.964737	-0.680549	0.841139
C	-1.066559	-1.455594	-0.163949
C	-0.312850	-0.144436	-0.547068
H	-4.007355	-0.246152	1.425465
H	-1.783579	-0.968429	1.881376
H	-2.243888	2.391659	-0.759611
H	-4.530739	1.085825	-0.513485
H	-3.532278	0.099702	-1.570136
H	-1.613471	-1.913683	-0.996476
H	-0.464060	0.126627	-1.600699
H	-0.783090	1.250990	1.168363
H	-3.904303	-1.518309	0.202628
H	-0.443964	-2.227875	0.297950
C	1.169867	-0.045204	-0.247466
C	2.011374	-1.165836	-0.320750
C	1.755571	1.197788	0.045448
C	3.387757	-1.052525	-0.101328
H	1.592283	-2.140012	-0.559082
C	3.129634	1.316535	0.266232
H	1.130556	2.086355	0.098183
C	3.953489	0.189286	0.196353
H	4.016663	-1.937557	-0.164024
H	3.556307	2.290707	0.493431
H	5.022791	0.278684	0.370505

6d-TSI

C	-1.427244	0.106563	0.944523
C	-2.217483	1.257953	0.932733
C	-3.365269	1.123168	-0.031779
C	-3.494163	-0.412120	-0.249695
C	-2.159600	-1.051771	0.230483
C	-1.085393	-1.327027	-0.844608
C	-0.263637	-0.050913	-0.654734
H	-4.319883	-0.796877	0.359747
H	-2.357298	-1.920456	0.869829
H	-1.946789	2.197310	1.407891
H	-4.294786	1.568298	0.347938
H	-3.149334	1.648497	-0.979552
H	-1.471810	-1.448829	-1.865801
H	-0.588516	0.784478	-1.274616
H	-0.705339	-0.086295	1.735923
H	-3.720703	-0.668579	-1.291454
H	-0.505750	-2.226207	-0.612039
C	1.166308	-0.021545	-0.358809
C	1.850428	-1.099945	0.248414
C	1.910538	1.152989	-0.621989
C	3.205586	-1.008767	0.564453
H	1.317886	-2.018966	0.477652
C	3.263664	1.243234	-0.304802
H	1.409402	1.999103	-1.088041
C	3.922875	0.161179	0.291196
H	3.705463	-1.856128	1.028098
H	3.808686	2.157937	-0.526130
H	4.979112	0.228724	0.538232

6d-TSII

C	-1.206701	0.768514	0.637207
C	-2.270001	1.529088	0.161971
C	-3.167297	0.815017	-0.813908
C	-3.485375	-0.559304	-0.116783
C	-2.315577	-0.999948	0.744153
C	-1.041348	-1.532187	0.112734
C	-0.387113	-0.187049	-0.271657
H	-4.368103	-0.431993	0.521192
H	-2.554184	-1.331971	1.753396

H	-2.681254	2.325285	0.780178
H	-4.084299	1.371063	-1.036241
H	-2.665937	0.634743	-1.775219
H	-1.202852	-2.220567	-0.731115
H	-0.636314	0.047214	-1.315717
H	-0.707543	1.082546	1.554627
H	-3.741735	-1.324036	-0.866159
H	-0.443446	-2.060420	0.863878
C	1.122017	-0.066290	-0.138588
C	1.956560	-1.191335	-0.215083
C	1.724315	1.194184	0.010325
C	3.347235	-1.064617	-0.139511
H	1.521725	-2.179507	-0.340875
C	3.112541	1.324993	0.088262
H	1.098943	2.082309	0.062787
C	3.931741	0.194257	0.015447
H	3.972119	-1.952494	-0.201475
H	3.554443	2.311698	0.205814
H	5.012459	0.294194	0.077511

6e

C	-1.453071	-0.734401	-0.800747
C	-1.480461	-1.366868	0.549181
C	-2.429154	-0.679140	1.487810
C	-3.352335	0.151836	0.557688
C	-2.505224	0.420307	-0.695136
C	-1.338775	1.443417	-0.564670
C	-0.341426	0.369172	-1.073716
H	-4.235576	-0.441496	0.286826
H	-3.105672	0.579577	-1.596582
H	-0.788365	-2.142776	0.864047
H	-2.990149	-1.381827	2.120398
H	-1.885597	-0.020400	2.190527
H	-1.165960	1.722068	0.481187
H	-0.243340	0.462478	-2.164293
H	-1.554271	-1.464032	-1.616770
H	-3.710650	1.075373	1.029684
H	-1.412966	2.362547	-1.156022
C	1.038257	0.216121	-0.479052
C	1.814696	-0.908109	-0.811684
C	1.596269	1.168146	0.384571
C	3.098715	-1.079079	-0.293687

H	1.404671	-1.658608	-1.485295
C	2.885551	1.003772	0.904475
H	1.026471	2.053793	0.652755
C	3.641150	-0.121074	0.570408
H	3.677878	-1.958806	-0.564726
H	3.296608	1.758718	1.570682
H	4.641765	-0.251213	0.974938

6e-TSI

C	-1.648522	-0.691875	0.985982
C	-1.675818	0.631675	1.435121
C	-2.399538	1.537179	0.471653
C	-3.256389	0.550011	-0.367009
C	-2.486933	-0.788452	-0.313304
C	-1.302673	-0.915389	-1.302389
C	-0.203129	-1.211870	-0.287375
H	-4.238438	0.431200	0.108081
H	-3.157054	-1.654714	-0.349177
H	-1.168287	0.993000	2.325130
H	-3.011519	2.293098	0.981394
H	-1.694032	2.100124	-0.163937
H	-1.129494	0.028178	-1.831598
H	-0.140310	-2.267120	-0.017263
H	-1.549178	-1.517123	1.689032
H	-3.427176	0.893999	-1.394651
H	-1.414087	-1.695808	-2.067363
C	1.087848	-0.533164	-0.215451
C	2.162125	-1.151823	0.465939
C	1.316486	0.752727	-0.753427
C	3.398344	-0.524677	0.598798
H	2.014672	-2.143689	0.889302
C	2.555960	1.379633	-0.623281
H	0.520191	1.267376	-1.283360
C	3.604881	0.748345	0.053147
H	4.205506	-1.029908	1.124071
H	2.704028	2.367874	-1.052652
H	4.569321	1.239593	0.152569

6e-TSII

C	-1.425327	-0.584639	-1.140411

C	-1.780798	-1.543176	-0.189437
C	-2.077399	-1.043060	1.196177
C	-3.092064	0.121906	0.944150
C	-2.609283	0.906842	-0.251669
C	-1.257966	1.590052	-0.131598
C	-0.410966	0.578571	-0.946114
H	-4.084890	-0.299945	0.744230
H	-3.350572	1.330311	-0.927162
H	-2.266953	-2.456969	-0.528037
H	-2.499307	-1.813387	1.850421
H	-1.178276	-0.653088	1.693873
H	-0.933950	1.659201	0.915055
H	-0.272571	1.009691	-1.947256
H	-1.561796	-0.881202	-2.182476
H	-3.181682	0.763741	1.835048
H	-1.239775	2.603878	-0.547488
C	0.977528	0.242046	-0.416531
C	1.519406	-1.049015	-0.495140
C	1.780605	1.263525	0.119297
C	2.819084	-1.312305	-0.050743
H	0.916094	-1.857959	-0.895443
C	3.078652	1.004524	0.565188
H	1.388476	2.275909	0.187888
C	3.604877	-0.288026	0.482293
H	3.214875	-2.322956	-0.119540
H	3.678118	1.812749	0.977740
H	4.614115	-0.493445	0.830367

6f

C	0.369255	0.489586	-0.602828
C	1.434304	1.451378	-0.219407
C	2.647565	0.752325	0.320424
C	2.536941	-0.684385	-0.254587
C	1.031124	-0.923338	-0.458106
C	0.169392	-1.201055	0.805770
C	-0.652871	0.090667	0.575027
H	3.051666	-0.730181	-1.222926
H	0.817378	-1.618351	-1.274820
H	1.288921	2.528057	-0.178009
H	3.586889	1.250255	0.043925
H	2.637855	0.731375	1.426682
H	0.741015	-1.182418	1.740652

H	-0.660364	0.816495	1.395702
H	-0.131412	0.735108	-1.548254
H	2.996083	-1.438973	0.395993
H	-0.426859	-2.116460	0.768066
C	-2.055832	-0.097968	0.038636
C	-2.958008	1.123864	0.067053
H	-3.250047	1.339030	1.103927
H	-2.431899	2.011566	-0.306174
H	-3.857014	0.944846	-0.527331
O	-2.436679	-1.159598	-0.431165

6f-TSI

C	0.559025	0.301879	-0.900319
C	1.368427	1.393179	-0.578409
C	2.461225	1.000840	0.377844
C	2.548616	-0.544624	0.229074
C	1.211169	-1.012341	-0.411191
C	0.087060	-1.449717	0.551769
C	-0.686656	-0.137298	0.588471
H	3.377785	-0.795472	-0.442554
H	1.394739	-1.738098	-1.211159
H	1.154742	2.423158	-0.852419
H	3.414667	1.498619	0.157860
H	2.200811	1.296285	1.409700
H	0.430118	-1.788381	1.537449
H	-0.437327	0.569985	1.378752
H	-0.118737	0.310449	-1.750842
H	2.746478	-1.046562	1.183180
H	-0.539392	-2.232669	0.114170
C	-2.060651	-0.047268	0.077988
C	-2.829077	1.230869	0.380813
H	-3.138257	1.241498	1.434802
H	-2.205135	2.119030	0.218745
H	-3.721549	1.286245	-0.247175
O	-2.564222	-0.944651	-0.603343

6f-TSII

C	0.261745	0.636506	-0.747579
C	1.348386	1.459957	-0.471727
C	2.285074	0.933745	0.582301

C	2.587416	-0.534835	0.117608
C	1.345496	-1.145360	-0.497637
C	0.147928	-1.467531	0.379872
C	-0.534861	-0.092058	0.379299
H	3.388307	-0.509007	-0.631166
H	1.480222	-1.723391	-1.410631
H	1.738874	2.109564	-1.253173
H	3.203677	1.522643	0.673647
H	1.817133	0.917865	1.576962
H	0.416619	-1.828045	1.383761
H	-0.391512	0.453094	1.322112
H	-0.266188	0.769494	-1.692973
H	2.953943	-1.141844	0.960018
H	-0.505296	-2.213500	-0.082584
C	-2.033026	-0.088132	0.079355
C	-2.749629	1.238106	0.261657
H	-2.932398	1.397667	1.333442
H	-2.139482	2.078291	-0.088721
H	-3.710993	1.222692	-0.257573
O	-2.625511	-1.087241	-0.291502

6g

C	-0.442176	0.011684	-1.104763
C	-0.752224	-1.345266	-0.577870
C	-1.807824	-1.310566	0.487021
C	-2.539731	0.036541	0.248953
C	-1.489721	0.947322	-0.408410
C	-0.367112	1.521899	0.503400
C	0.715171	0.849879	-0.370145
H	-3.381053	-0.117101	-0.439372
H	-1.932266	1.703296	-1.064986
H	-0.182949	-2.236813	-0.827846
H	-2.485698	-2.174119	0.445936
H	-1.348982	-1.333642	1.491964
H	-0.378955	1.107076	1.516352
H	-0.352975	0.043252	-2.198539
H	-2.945284	0.467329	1.172604
H	-0.309040	2.612937	0.573899
C	1.804322	0.042595	0.301758
O	1.762206	-0.242119	1.488640
C	2.942187	-0.431146	-0.585977
H	2.554491	-0.915684	-1.491219

H	3.539070	0.429734	-0.916093
H	3.584430	-1.125694	-0.039496
H	1.164209	1.538740	-1.096126

6g-TSI

C	0.658082	0.050280	1.225362
C	0.914422	-1.271493	0.849493
C	1.751007	-1.344122	-0.398859
C	2.421581	0.054788	-0.460560
C	1.465459	1.000407	0.304778
C	0.278659	1.564080	-0.513357
C	-0.862275	0.951405	0.286192
H	3.390269	0.016010	0.053713
H	2.009809	1.779296	0.850280
H	0.484708	-2.145007	1.332630
H	2.482302	-2.162280	-0.368754
H	1.111862	-1.526370	-1.277666
H	0.266598	1.183879	-1.540021
H	0.397371	0.304299	2.250931
H	2.605863	0.394089	-1.486334
H	0.237066	2.659196	-0.552955
C	-1.790132	-0.014091	-0.314530
O	-1.555460	-0.557784	-1.396486
C	-3.037688	-0.367205	0.482362
H	-2.789460	-0.591676	1.527702
H	-3.733832	0.482262	0.491243
H	-3.535869	-1.228159	0.030303
H	-1.277697	1.552441	1.095528

6g-TSII

C	0.531626	-0.337237	1.248794
C	1.269777	-1.313176	0.576056
C	1.715575	-0.984936	-0.819301
C	2.347826	0.439479	-0.673052
C	1.470416	1.248570	0.251640
C	0.045264	1.519402	-0.204653
C	-0.666785	0.453147	0.679802
H	3.354798	0.347631	-0.247354
H	1.942217	1.971207	0.915129
H	1.849773	-2.024421	1.160813

H	2.435333	-1.706329	-1.220305
H	0.870299	-0.952967	-1.520309
H	-0.078659	1.331710	-1.279970
H	0.519746	-0.420211	2.337432
H	2.452484	0.924967	-1.656591
H	-0.299513	2.540384	-0.007515
C	-1.772481	-0.328018	-0.029998
O	-1.683499	-1.509251	-0.311562
C	-3.015545	0.476873	-0.385146
H	-3.588037	0.682538	0.529669
H	-2.757033	1.446805	-0.826493
H	-3.644242	-0.091660	-1.074594
H	-1.143210	0.979720	1.517720

7a

C	1.153800	-1.118711	0.874570
C	2.066098	-0.446080	-0.164592
C	1.687118	1.029755	-0.358297
C	0.242182	1.151628	-0.866456
C	-0.796630	0.541697	0.107243
C	-0.337888	-0.885552	0.620501
C	-1.927587	-0.229481	-0.684548
C	-1.088391	-1.528227	-0.576192
C	-1.227060	1.507018	1.144160
H	3.113411	-0.537574	0.152007
H	1.988073	-0.965291	-1.131689
H	2.371801	1.507629	-1.071603
H	1.797911	1.567560	0.595310
H	0.182546	0.644918	-1.839740
H	-0.018021	2.202016	-1.055692
H	-0.897243	-1.113623	1.537754
H	1.402035	-0.711155	1.866006
H	1.356382	-2.198635	0.924271
H	-2.168380	0.157332	-1.681844
H	-2.850630	-0.291888	-0.097602
H	-1.625291	-2.463323	-0.383035
H	-0.442473	-1.676263	-1.448979
H	-1.866431	1.183027	1.962474
H	-0.973552	2.562993	1.094022

7a-TSI

C	-0.390448	-0.775739	0.671547
C	1.092201	-1.100680	0.927612
C	2.025850	-0.571881	-0.174950
C	1.783750	0.921071	-0.448112
C	0.318843	1.178508	-0.858203
C	-0.640597	0.684188	0.226240
C	-1.187071	1.611869	1.100194
C	-1.117158	-1.494535	-0.485838
C	-2.086899	-0.376839	-0.819992
H	3.070954	-0.741145	0.116003
H	1.871160	-1.138227	-1.105396
H	2.455567	1.275366	-1.241538
H	2.018950	1.503729	0.454237
H	0.139296	0.666979	-1.812887
H	0.151367	2.247372	-1.039600
H	-0.957312	-0.951875	1.595567
H	1.385300	-0.642702	1.883646
H	1.217487	-2.186193	1.048571
H	-2.198175	-0.013607	-1.840517
H	-2.987149	-0.300947	-0.213433
H	-1.583373	-2.448655	-0.205482
H	-0.441713	-1.694892	-1.325528
H	-1.700623	1.299834	2.007130
H	-1.232554	2.669189	0.848244

7a-TSII

C	1.549224	-1.334290	1.117181
C	1.021696	-0.618779	0.050539
C	1.846691	0.474782	-0.651952
C	0.817016	1.617936	-0.608248
C	0.100591	1.149595	0.647708
C	-1.394920	1.084455	0.798540
C	-2.098250	0.156074	-0.210942
C	-1.494507	-1.254031	-0.247836
C	-0.060719	-1.290648	-0.810647
H	-3.162865	0.098254	0.052068
H	-2.055788	0.591745	-1.220179
H	-2.127373	-1.900086	-0.871405
H	-1.506556	-1.687863	0.762840
H	-0.072635	-0.825650	-1.806119
H	0.232122	-2.336750	-0.972514

H	0.642953	1.372544	1.567233
H	-1.628438	0.738076	1.815103
H	-1.828094	2.098654	0.715805
H	2.198850	0.183856	-1.652140
H	2.727501	0.722368	-0.047297
H	1.241583	2.630273	-0.550455
H	0.154465	1.589955	-1.481054
H	2.420295	-0.977209	1.661324
H	1.043052	-2.208730	1.520742

7b

C	0.931546	-0.963655	-1.349252
C	2.453292	-1.168810	-1.342287
C	2.996014	-1.185596	0.091016
C	2.738324	0.167764	0.762787
C	1.236897	0.549283	0.894025
C	0.412646	0.214351	-0.491535
C	1.021519	2.053106	0.521042
C	0.807566	1.648695	-0.951705
C	0.686362	0.098971	2.190052
H	2.687193	-2.108524	-1.859853
H	2.957881	-0.371618	-1.907612
H	4.073585	-1.397012	0.090975
H	2.517421	-1.996312	0.661740
H	3.262980	0.935031	0.177297
H	3.189437	0.196133	1.763172
H	0.467578	-1.892628	-0.995588
H	0.568208	-0.819489	-2.377740
H	1.848138	2.732659	0.760073
H	0.101445	2.444214	0.968481
H	0.092323	2.224743	-1.544150
H	1.750693	1.631578	-1.507289
H	-0.269828	0.466355	2.549306
H	1.182217	-0.666572	2.782147
C	-1.088646	0.021039	-0.255072
C	-1.536211	-1.106829	0.461520
C	-2.070154	0.886829	-0.759258
C	-2.892734	-1.352306	0.671613
H	-0.808394	-1.803863	0.868079
C	-3.434661	0.645866	-0.554872
H	-1.785920	1.766398	-1.326591
C	-3.854526	-0.473279	0.162667

H	-3.199157	-2.231465	1.233753
H	-4.166016	1.339554	-0.963137
H	-4.913187	-0.661753	0.322491

7b-TSI

C	0.430761	0.152994	-0.434096
C	0.974037	-1.072675	-1.226526
C	2.504161	-1.213597	-1.244587
C	3.084278	-1.142776	0.173016
C	2.721429	0.201153	0.828597
C	1.202246	0.397561	0.923034
C	0.624479	0.243052	2.173293
C	0.811490	1.515591	-1.069291
C	0.946637	2.328126	0.199132
H	2.766722	-2.166567	-1.722711
H	2.962224	-0.427210	-1.861601
H	4.176202	-1.257385	0.147074
H	2.689713	-1.970736	0.779741
H	3.192703	0.997863	0.239229
H	3.150261	0.266776	1.835704
H	0.560468	-1.991668	-0.796175
H	0.582287	-1.014207	-2.251773
H	1.820678	2.953711	0.373297
H	0.033211	2.681465	0.671166
H	0.111100	1.901119	-1.819772
H	1.780692	1.433265	-1.570312
H	-0.449183	0.201679	2.319609
H	1.239290	0.303575	3.068518
C	-1.084985	-0.024245	-0.230270
C	-1.574356	-1.192763	0.386789
C	-2.036532	0.919763	-0.645709
C	-2.939772	-1.411539	0.569221
H	-0.875831	-1.941489	0.748688
C	-3.408926	0.706853	-0.467627
H	-1.724073	1.845205	-1.116600
C	-3.870108	-0.461141	0.137772
H	-3.276384	-2.326319	1.051440
H	-4.113837	1.462178	-0.807005
H	-4.935279	-0.629402	0.274985

7b-TSII

C	0.652866	0.608806	2.137171
C	1.298742	0.825429	0.905017
C	0.987609	2.086628	0.073804
C	0.807736	1.373280	-1.273059
C	0.349107	0.036106	-0.671645
C	0.985967	-1.240549	-1.209423
C	2.509948	-1.368181	-1.047873
C	2.969513	-1.115085	0.390620
C	2.761693	0.346822	0.813505
H	2.803965	-2.376546	-1.368409
H	3.032753	-0.672027	-1.719570
H	4.035676	-1.361578	0.486180
H	2.431933	-1.785578	1.077742
H	3.307336	0.984912	0.104679
H	3.235867	0.512908	1.789969
H	0.520589	-2.110631	-0.733710
H	0.726366	-1.315584	-2.280397
H	1.771985	2.854560	0.119558
H	0.049188	2.540612	0.409936
H	0.128179	1.844631	-1.993242
H	1.768916	1.248428	-1.782978
H	-0.307856	1.063127	2.361443
H	1.020761	-0.132705	2.843661
C	-1.103678	-0.099078	-0.346268
C	-1.558852	-1.164824	0.461251
C	-2.074769	0.813271	-0.802255
C	-2.906500	-1.318714	0.779766
H	-0.841905	-1.873948	0.864882
C	-3.428684	0.660281	-0.488009
H	-1.782724	1.653584	-1.423194
C	-3.855217	-0.407168	0.303056
H	-3.217257	-2.150150	1.408274
H	-4.149468	1.380663	-0.867953
H	-4.907198	-0.526818	0.549166

7c

C	0.432668	-1.528018	-0.631788
C	1.963407	-1.404563	-0.647717
C	2.456136	-0.572829	0.541332
C	1.909992	0.856536	0.440222
C	0.361914	0.963068	0.472372

C	-0.321598	-0.192035	-0.477050
C	-0.144623	1.980654	-0.606711
C	-0.270853	0.836147	-1.637130
C	-0.142918	1.137171	1.852288
H	2.401015	-2.411115	-0.628530
H	2.304473	-0.935595	-1.581616
H	3.553373	-0.545467	0.560708
H	2.136404	-1.042482	1.484147
H	2.283129	1.288713	-0.497903
H	2.313966	1.485680	1.244013
H	0.169451	-2.199385	0.194589
H	0.081155	-2.018109	-1.551916
H	0.540527	2.806786	-0.828226
H	-1.124840	2.391043	-0.347392
H	-1.146516	0.855253	-2.289703
H	0.632731	0.716889	-2.243855
H	-1.174028	1.428323	2.035752
H	0.485524	0.949273	2.719206
C	-1.771003	-0.443011	-0.036630
C	-2.039124	-1.413603	1.105945
H	-2.136162	-2.431243	0.704825
H	-1.239511	-1.420149	1.852431
H	-2.988431	-1.146788	1.577337
O	-2.712031	0.113908	-0.581833

7c-TSI

C	-0.305946	-0.128849	-0.415537
C	0.443886	-1.459741	-0.697088
C	1.971174	-1.316725	-0.781686
C	2.526189	-0.607820	0.459664
C	1.910795	0.796315	0.590610
C	0.381904	0.746833	0.697587
C	-0.181079	0.976207	1.943085
C	-0.250450	0.920431	-1.551557
C	-0.216872	2.170758	-0.699398
H	2.416472	-2.314272	-0.889895
H	2.256764	-0.752326	-1.680622
H	3.619165	-0.525102	0.396159
H	2.301560	-1.199811	1.358764
H	2.227183	1.381456	-0.281954
H	2.309932	1.311864	1.472371
H	0.224862	-2.179612	0.100555

H	0.049751	-1.892168	-1.627824
H	0.559925	2.921567	-0.831147
H	-1.171111	2.551140	-0.345233
H	-1.103285	0.864777	-2.235936
H	0.669341	0.811356	-2.134875
H	-1.238171	0.831776	2.145783
H	0.391468	1.480240	2.718056
C	-1.774893	-0.432781	-0.045799
C	-2.075905	-1.537878	0.957350
H	-2.156511	-2.493698	0.422474
H	-1.301993	-1.645051	1.722131
H	-3.042541	-1.334204	1.425465
O	-2.698203	0.177695	-0.559707

7c-TSII

C	0.122241	-1.389608	1.733381
C	-0.434982	-1.152684	0.456302
C	0.108416	-1.896594	-0.782088
C	0.254841	-0.665320	-1.690804
C	0.393647	0.345653	-0.546056
C	-0.417457	1.632452	-0.558136
C	-1.945437	1.463942	-0.532672
C	-2.405096	0.564978	0.617568
C	-1.953730	-0.889630	0.420274
H	-2.399485	2.459420	-0.443107
H	-2.305117	1.046023	-1.483536
H	-3.500625	0.584414	0.688076
H	-2.023977	0.955604	1.573042
H	-2.351753	-1.237915	-0.542196
H	-2.420455	-1.523285	1.185797
H	-0.138637	2.253594	0.300279
H	-0.132432	2.207401	-1.456300
H	-0.563141	-2.689603	-1.136423
H	1.085956	-2.338208	-0.571576
H	1.114380	-0.687447	-2.368190
H	-0.650556	-0.475465	-2.277355
H	1.129340	-1.782494	1.843906
H	-0.389594	-1.072953	2.639765
C	1.785079	0.452110	-0.008611
C	2.079521	1.420753	1.128187
H	2.147344	2.448843	0.748848
H	1.299920	1.402261	1.897890

H	3.041786	1.154362	1.571631
O	2.691848	-0.252608	-0.449328

7d

C	-2.807452	1.394172	0.473252
C	-3.816405	0.423412	-0.161645
C	-3.480854	-1.031821	0.197294
C	-2.084661	-1.403905	-0.325221
C	-0.960862	-0.517432	0.268735
C	-1.344956	1.010381	0.226354
C	0.121815	-0.173847	-0.892965
C	-0.687885	1.123944	-1.171269
C	-0.473996	-1.038466	1.562531
H	-4.830915	0.678814	0.171306
H	-3.813516	0.532457	-1.256657
H	-4.228640	-1.712015	-0.231754
H	-3.522919	-1.162624	1.288830
H	-2.099763	-1.306649	-1.419586
H	-1.857128	-2.458244	-0.116759
H	-0.716646	1.541804	0.952109
H	-2.979750	1.407302	1.559736
H	-2.984383	2.420420	0.119740
H	0.080931	-0.918365	-1.696025
H	-0.116728	2.034060	-1.382665
H	-1.402649	0.978389	-1.988298
H	0.196146	-0.447897	2.181170
H	-0.674473	-2.059772	1.877060
C	1.561517	-0.029798	-0.459823
C	2.420001	-1.136407	-0.582496
C	2.094329	1.149751	0.084524
C	3.753370	-1.074043	-0.174434
H	2.033895	-2.060595	-1.008492
C	3.429313	1.219086	0.494781
H	1.469761	2.032571	0.188639
C	4.265777	0.107748	0.369062
H	4.393006	-1.946438	-0.285634
H	3.815029	2.147227	0.910146
H	5.304433	0.162900	0.685055

7d-TSI

C	-2.833697	1.394834	0.427043
C	-3.817345	0.443910	-0.276212
C	-3.560303	-1.018494	0.120286
C	-2.122897	-1.436875	-0.244849
C	-1.090701	-0.537381	0.448359
C	-1.362492	0.977928	0.266377
C	0.221412	-0.121921	-0.963010
C	-0.679407	1.107693	-1.110246
C	-0.545512	-1.014668	1.653305
H	-4.847321	0.732683	-0.028936
H	-3.724422	0.541684	-1.368302
H	-4.276204	-1.680544	-0.385171
H	-3.717879	-1.141926	1.201396
H	-2.028496	-1.382289	-1.337802
H	-1.942029	-2.483337	0.031644
H	-0.760839	1.522101	1.005451
H	-3.071660	1.409510	1.500748
H	-2.968268	2.423922	0.063944
H	0.078216	-0.922019	-1.689129
H	-0.152892	2.053734	-1.284097
H	-1.384560	0.972425	-1.937819
H	0.012989	-0.360260	2.317954
H	-0.520918	-2.078878	1.877561
C	1.615500	-0.009922	-0.517147
C	2.477202	-1.119780	-0.657761
C	2.142642	1.148897	0.089922
C	3.798269	-1.075714	-0.217813
H	2.096081	-2.026368	-1.123958
C	3.466576	1.195088	0.530103
H	1.516044	2.027652	0.214866
C	4.302927	0.084827	0.380536
H	4.438028	-1.945963	-0.344371
H	3.847126	2.104102	0.990177
H	5.333961	0.123247	0.722479

7d-TSII

C	-2.867107	1.503321	0.377549
C	-3.796933	0.431014	-0.222654
C	-3.455314	-0.987423	0.252225
C	-2.101355	-1.495858	-0.276096
C	-0.845636	-0.796710	0.274997
C	-1.397621	1.219679	0.217984

C	0.098126	-0.219159	-0.830638
C	-0.701809	1.073392	-1.123628
C	-0.386717	-1.179428	1.524001
H	-4.832279	0.676289	0.048911
H	-3.753880	0.461777	-1.321534
H	-4.238468	-1.679044	-0.086999
H	-3.463936	-1.022868	1.351430
H	-2.113053	-1.412732	-1.371523
H	-2.013815	-2.568932	-0.058978
H	-0.771238	1.633415	1.007035
H	-3.088972	1.597804	1.449675
H	-3.113925	2.483787	-0.070889
H	0.097078	-0.907018	-1.688035
H	-0.091077	1.934193	-1.429093
H	-1.427365	0.896402	-1.925251
H	0.579335	-0.863281	1.904781
H	-1.034357	-1.719244	2.211667
C	1.549574	-0.036043	-0.420620
C	2.448495	-1.096439	-0.624723
C	2.047357	1.137292	0.166153
C	3.791030	-0.994878	-0.256068
H	2.086961	-2.016174	-1.080479
C	3.391611	1.246509	0.537216
H	1.388652	1.983999	0.336836
C	4.269914	0.181065	0.329148
H	4.463186	-1.831813	-0.429922
H	3.750283	2.168826	0.988078
H	5.315195	0.266613	0.615215

7e

C	-3.309313	-0.565556	-0.517362
C	-3.146216	-1.073589	0.924400
C	-2.439137	-0.028485	1.799680
C	-1.034641	0.273457	1.253718
C	-1.062081	0.836758	-0.186483
C	-2.017606	-0.007987	-1.120530
C	0.126131	0.238433	-1.094359
C	-0.820701	-0.920809	-1.489026
C	-1.243135	2.302993	-0.211320
H	-4.131685	-1.322423	1.339475
H	-2.561406	-2.005642	0.936025
H	-2.361105	-0.389817	2.833684

H	-3.040167	0.892786	1.831786
H	-0.450179	-0.654889	1.286303
H	-0.506133	0.979318	1.907209
H	-2.267658	0.603982	-1.997323
H	-4.062577	0.236272	-0.517756
H	-3.704806	-1.361513	-1.165072
H	0.225061	0.912849	-1.954648
H	-0.761707	-1.289652	-2.518956
H	-0.739120	-1.776396	-0.809818
H	-1.409846	2.819549	-1.154389
H	-1.167695	2.910365	0.686974
C	1.493210	0.011827	-0.501166
C	2.291961	1.119310	-0.162718
C	2.016904	-1.269607	-0.277911
C	3.562746	0.952163	0.388080
H	1.907094	2.122727	-0.334644
C	3.293958	-1.442552	0.267811
H	1.430787	-2.145794	-0.541728
C	4.071076	-0.333458	0.606140
H	4.159836	1.824655	0.643043
H	3.679402	-2.447217	0.425351
H	5.062957	-0.466545	1.030749

7e-TSI

C	-3.283058	-0.214484	-0.773012
C	-3.107432	-1.422717	0.162752
C	-2.490410	-1.003297	1.505527
C	-1.114620	-0.339334	1.296769
C	-1.226139	0.884046	0.385027
C	-2.002188	0.619959	-0.931271
C	0.249100	0.794944	-0.919611
C	-0.807501	0.032844	-1.709900
C	-1.314044	2.140610	1.012226
H	-4.079235	-1.907921	0.322652
H	-2.461445	-2.177648	-0.309822
H	-2.379100	-1.877417	2.161007
H	-3.165247	-0.303089	2.018933
H	-0.434233	-1.088845	0.873624
H	-0.679259	-0.041773	2.258523
H	-2.262459	1.589359	-1.377287
H	-4.069037	0.434641	-0.359960
H	-3.635258	-0.541178	-1.761931

H	0.294149	1.848701	-1.193817
H	-0.802062	0.216394	-2.792592
H	-0.729351	-1.048664	-1.558466
H	-1.631497	3.023893	0.461828
H	-0.935822	2.297004	2.019896
C	1.544531	0.263731	-0.495603
C	2.514634	1.148224	0.032238
C	1.879379	-1.106762	-0.557088
C	3.750106	0.687872	0.478691
H	2.282012	2.209770	0.087236
C	3.121032	-1.566960	-0.115129
H	1.172278	-1.818405	-0.973495
C	4.062556	-0.676013	0.408192
H	4.475936	1.392508	0.877823
H	3.355125	-2.626741	-0.184234
H	5.028832	-1.036560	0.751242

7e-TSII

C	-3.322102	-0.958712	-0.203366
C	-3.115219	-0.643424	1.291137
C	-2.547244	0.761508	1.532029
C	-1.099544	0.930208	1.033935
C	-0.906368	0.895116	-0.490639
C	-2.114772	-0.713531	-1.065970
C	0.098343	-0.153933	-1.036917
C	-0.780355	-1.410506	-0.881979
C	-1.179906	2.046123	-1.214407
H	-4.079874	-0.748707	1.805081
H	-2.443319	-1.385462	1.746890
H	-2.566788	0.976138	2.609115
H	-3.196508	1.509461	1.053587
H	-0.481617	0.152280	1.500318
H	-0.703720	1.883303	1.407945
H	-2.334439	-0.449288	-2.100592
H	-4.150821	-0.342986	-0.579808
H	-3.652472	-2.009108	-0.306474
H	0.204132	0.047154	-2.113124
H	-0.574282	-2.216497	-1.600507
H	-0.691146	-1.834793	0.124847
H	-0.930361	2.123931	-2.270253
H	-1.761870	2.860375	-0.787542
C	1.489542	-0.146660	-0.422468

C	2.187472	1.063076	-0.265521
C	2.127984	-1.332597	-0.032224
C	3.477346	1.086325	0.267250
H	1.707830	1.993815	-0.559696
C	3.422448	-1.314216	0.498971
H	1.616889	-2.284964	-0.146406
C	4.102202	-0.104522	0.652605
H	3.995737	2.035490	0.381941
H	3.896701	-2.247778	0.792645
H	5.106968	-0.087889	1.067423

7f

C	2.078353	-1.237943	0.631412
C	2.991907	-0.375131	-0.254148
C	2.611203	1.109827	-0.156768
C	1.167159	1.323591	-0.636537
C	0.137099	0.531241	0.206582
C	0.585225	-0.964164	0.430595
C	-1.001137	-0.079889	-0.780565
C	-0.162658	-1.378345	-0.861211
C	-0.283502	1.278482	1.411353
H	4.038426	-0.524260	0.041798
H	2.918251	-0.695730	-1.304119
H	3.293557	1.720171	-0.762945
H	2.718985	1.452184	0.883168
H	1.113245	1.008769	-1.687385
H	0.901569	2.389448	-0.621937
H	0.026258	-1.365959	1.282919
H	2.328037	-1.036613	1.683840
H	2.278080	-2.306431	0.466640
H	-1.106448	0.506991	-1.700667
H	-0.729225	-2.311968	-0.810841
H	0.477974	-1.390254	-1.749445
H	-0.839045	0.784360	2.204366
H	-0.089416	2.342770	1.519680
C	-2.357751	-0.226238	-0.121011
C	-3.328768	0.923556	-0.316977
H	-2.845000	1.880088	-0.082529
H	-3.640974	0.969783	-1.369188
H	-4.209572	0.786023	0.314560
O	-2.657186	-1.204912	0.546968

7f-TSI

C	2.073839	-1.243061	0.620785
C	2.975685	-0.436373	-0.328265
C	2.682132	1.068772	-0.232482
C	1.209956	1.360387	-0.587492
C	0.265288	0.596816	0.349709
C	0.579735	-0.916970	0.469159
C	-1.109191	-0.157169	-0.856149
C	-0.171454	-1.359088	-0.803668
C	-0.237132	1.303897	1.457001
H	4.029320	-0.635267	-0.093413
H	2.823805	-0.765967	-1.366876
H	3.338425	1.630046	-0.910652
H	2.894954	1.424779	0.785774
H	1.055343	1.067345	-1.633448
H	1.000688	2.435887	-0.527879
H	0.033766	-1.312379	1.332474
H	2.371764	-1.023395	1.656691
H	2.227340	-2.321324	0.474674
H	-1.103242	0.485752	-1.736011
H	-0.692368	-2.316890	-0.708491
H	0.474292	-1.396031	-1.687784
H	-0.718274	0.786394	2.283037
H	-0.272332	2.391330	1.462935
C	-2.409004	-0.239308	-0.163348
C	-3.386260	0.901753	-0.392954
H	-2.926444	1.856767	-0.105376
H	-3.654016	0.978267	-1.454701
H	-4.290462	0.741493	0.198770
O	-2.679264	-1.163094	0.604563

7f-TSII

C	2.165002	-1.328033	0.564094
C	2.974377	-0.345210	-0.303927
C	2.572848	1.118691	-0.081992
C	1.156417	1.448560	-0.590163
C	-0.005089	0.789224	0.173254
C	0.673167	-1.176154	0.460124
C	-0.959584	-0.056948	-0.729246
C	-0.110648	-1.339053	-0.828734

C	-0.415138	1.369659	1.362618
H	4.040497	-0.475847	-0.076160
H	2.857199	-0.592877	-1.369389
H	3.284099	1.771519	-0.605905
H	2.652093	1.366815	0.986477
H	1.102904	1.167894	-1.650765
H	1.010202	2.536710	-0.559231
H	0.111377	-1.464690	1.346498
H	2.458046	-1.192501	1.614426
H	2.454653	-2.362120	0.300167
H	-1.112475	0.457523	-1.690000
H	-0.703132	-2.260941	-0.877447
H	0.539418	-1.301853	-1.709939
H	-1.293021	1.028189	1.903695
H	0.224667	2.082053	1.878479
C	-2.336167	-0.270435	-0.102476
C	-3.374426	0.803010	-0.370888
H	-2.947840	1.804036	-0.240394
H	-3.710579	0.726200	-1.414379
H	-4.235057	0.668927	0.288915
O	-2.597201	-1.254862	0.569872

7g

C	-2.471486	-0.694532	-0.606705
C	-2.641559	-0.398743	0.891683
C	-1.966168	0.927583	1.267969
C	-0.456753	0.858041	0.986785
C	-0.142871	0.608535	-0.508313
C	-1.027420	-0.564158	-1.099664
C	1.091422	-0.422077	-0.712862
C	0.074951	-1.580152	-0.709518
C	-0.092558	1.858541	-1.291530
H	-3.710288	-0.372534	1.140956
H	-2.201254	-1.207715	1.492744
H	-2.128207	1.149440	2.330751
H	-2.423064	1.751456	0.699149
H	-0.037250	0.053706	1.602266
H	0.040615	1.782145	1.311123
H	-1.032541	-0.464212	-2.193234
H	-3.094484	0.014607	-1.171918
H	-2.848755	-1.698677	-0.848129
H	1.498957	-0.248007	-1.716402

H	0.262106	-2.407952	-1.401346
H	-0.047839	-1.987430	0.298330
H	-0.001520	1.825502	-2.375080
H	-0.119768	2.837271	-0.819393
C	2.214086	-0.382160	0.297252
C	3.277055	0.681277	0.087770
H	3.900567	0.412796	-0.775999
H	2.819840	1.652353	-0.140529
H	3.911837	0.760814	0.973566
O	2.257356	-1.150812	1.246993

7g-TSI

C	-2.435200	-0.445888	-0.860814
C	-2.608352	-0.791805	0.626931
C	-2.035371	0.316656	1.522225
C	-0.531726	0.519090	1.246245
C	-0.290523	0.884265	-0.220171
C	-0.995464	-0.058752	-1.233123
C	1.229006	-0.180183	-0.876600
C	0.106271	-1.135666	-1.247587
C	-0.118472	2.248052	-0.528913
H	-3.672567	-0.949209	0.845205
H	-2.100672	-1.739113	0.858744
H	-2.175165	0.061128	2.580529
H	-2.580329	1.255708	1.345348
H	-0.009631	-0.406880	1.511991
H	-0.123688	1.306252	1.892694
H	-1.005821	0.439629	-2.211994
H	-3.094219	0.401591	-1.101221
H	-2.760791	-1.283765	-1.493249
H	1.599238	0.441838	-1.691537
H	0.242338	-1.661547	-2.200589
H	-0.021470	-1.883112	-0.458846
H	-0.177830	2.605036	-1.554724
H	0.198058	2.962990	0.227182
C	2.226355	-0.486835	0.158550
C	3.419487	0.449265	0.268527
H	4.111928	0.272589	-0.565677
H	3.106690	1.499486	0.210554
H	3.948485	0.269925	1.207686
O	2.089923	-1.437717	0.933285

7g-TSII

C	2.543974	-0.795842	0.592454
C	2.635840	-0.382167	-0.889700
C	1.997318	0.984856	-1.166356
C	0.465436	0.986445	-1.000636
C	-0.054806	0.817748	0.436608
C	1.159923	-0.723260	1.175386
C	-1.034716	-0.368415	0.683987
C	-0.025503	-1.522179	0.666776
C	-0.086406	1.930892	1.262285
H	3.694476	-0.364680	-1.180080
H	2.154451	-1.138712	-1.525802
H	2.228706	1.287556	-2.196340
H	2.445632	1.744708	-0.509464
H	0.054098	0.195137	-1.639293
H	0.067667	1.929859	-1.398022
H	1.122376	-0.508574	2.243777
H	3.207193	-0.146490	1.180592
H	2.941913	-1.821164	0.705020
H	-1.449429	-0.237849	1.693153
H	-0.304579	-2.387302	1.283888
H	0.120981	-1.881750	-0.356203
H	-0.569967	1.904259	2.236001
H	0.480481	2.827687	1.022023
C	-2.202697	-0.441806	-0.297697
C	-3.321923	0.563864	-0.105542
H	-3.905139	0.292804	0.785434
H	-2.921568	1.569411	0.068823
H	-3.983051	0.562101	-0.975537
O	-2.230361	-1.265978	-1.197921

8a

C	-0.560392	0.856034	-0.519422
C	0.771729	1.454486	-0.256448
C	1.890442	0.647901	0.332461
C	1.815709	-0.838960	-0.067783
C	0.420132	-1.408460	0.226827
C	-0.664104	-0.702958	-0.602890
C	-2.048902	-0.615609	0.097414
C	-1.678840	0.805995	0.598779

H	2.859360	1.077160	0.041364
H	1.868756	0.705606	1.439780
H	2.583206	-1.408465	0.472347
H	2.037880	-0.941268	-1.140104
H	0.211409	-1.283850	1.300658
H	0.388234	-2.489092	0.032033
H	-1.011110	1.311756	-1.412618
H	0.895818	2.532026	-0.356576
H	-2.271991	-1.376321	0.855095
H	-2.874284	-0.590769	-0.623325
H	-2.450398	1.582330	0.556306
H	-1.247455	0.796778	1.605334
H	-0.664067	-1.106466	-1.623917

8a-TSI

C	-0.645957	-0.605325	-0.652572
C	-0.371801	0.906697	-0.624959
C	0.855919	1.433458	-0.259860
C	1.937483	0.598784	0.372408
C	1.803639	-0.887365	-0.004805
C	0.365104	-1.374557	0.218223
C	-1.891345	0.706598	0.779314
C	-2.059359	-0.566646	-0.033476
H	2.923710	0.982021	0.075650
H	1.904472	0.697265	1.473206
H	2.506854	-1.491593	0.583116
H	2.076734	-1.018430	-1.061902
H	0.112189	-1.243708	1.281005
H	0.278940	-2.449520	0.010610
H	-0.993028	1.505975	-1.291137
H	1.024444	2.505780	-0.351972
H	-2.330699	-1.461234	0.545456
H	-2.822766	-0.429803	-0.809019
H	-2.622339	1.509985	0.706047
H	-1.405034	0.632600	1.749762
H	-0.615577	-1.009200	-1.676457

8a-TSII

C	0.745080	0.907735	-0.662328
C	0.561426	-1.170117	-0.472138

C	-0.796461	-1.441923	-0.420319
C	-1.717486	-0.674227	0.486967
C	-1.782896	0.795212	-0.005911
C	-0.420029	1.522040	0.094983
C	1.489735	-0.787620	0.688611
C	1.996257	0.553831	0.129511
H	-2.724531	-1.109185	0.479755
H	-1.374506	-0.685741	1.531217
H	-2.522315	1.353870	0.584433
H	-2.134386	0.806395	-1.047449
H	-0.156779	1.594630	1.160763
H	-0.563509	2.559667	-0.247775
H	1.101628	-1.577183	-1.329735
H	-1.253569	-1.878534	-1.308828
H	2.294471	1.295617	0.886143
H	2.850840	0.398519	-0.540165
H	2.260703	-1.543934	0.890040
H	0.921949	-0.642506	1.613843
H	0.846245	1.198800	-1.708502

8b

C	1.470583	0.307271	-1.062534
C	2.292829	-0.926754	-1.022442
C	2.653415	-1.580690	0.276964
C	1.542839	-1.425011	1.334954
C	1.119973	0.044296	1.464459
C	0.515154	0.610875	0.149901
C	0.859310	2.125987	-0.018771
C	2.119648	1.727858	-0.825170
H	2.887818	-2.641813	0.115400
H	3.583098	-1.136372	0.687303
H	1.898376	-1.797971	2.304115
H	0.676753	-2.040015	1.056676
H	2.004830	0.636657	1.740539
H	0.394435	0.172103	2.277979
H	0.904950	0.359502	-2.002560
H	2.781173	-1.262300	-1.936309
H	1.008113	2.707512	0.898759
H	0.121969	2.639053	-0.645594
H	2.351103	2.309322	-1.723260
H	3.019075	1.668425	-0.204313
C	-0.941438	0.212793	0.003424

C	-1.940693	0.942795	0.669076
C	-1.336157	-0.889724	-0.769292
C	-3.286756	0.585629	0.567296
H	-1.660951	1.805402	1.270767
C	-2.682840	-1.253290	-0.872987
H	-0.583919	-1.470240	-1.297816
C	-3.664336	-0.517257	-0.205370
H	-4.041269	1.170430	1.088377
H	-2.963020	-2.111849	-1.478971
H	-4.711724	-0.796522	-0.288148

8b-TSI

C	-3.671576	-0.469539	-0.166026
C	-3.244054	0.597778	0.630461
C	-1.888583	0.924592	0.696716
C	-0.926460	0.198761	-0.027814
C	-1.371465	-0.867161	-0.823216
C	-2.728833	-1.199959	-0.891845
C	0.548716	0.577222	0.083533
C	1.424836	0.097230	-1.091867
C	2.263565	-0.998032	-1.010153
C	2.607507	-1.667860	0.292438
C	1.527471	-1.428153	1.361142
C	1.148791	0.056810	1.421367
C	2.201254	2.005162	-0.724384
C	0.838173	2.098640	-0.071519
H	2.756551	-2.744518	0.130186
H	3.578021	-1.291449	0.665483
H	1.887111	-1.763297	2.342489
H	0.637824	-2.028032	1.127440
H	2.051528	0.637568	1.659522
H	0.433100	0.244802	2.231232
H	1.063554	0.379937	-2.080775
H	2.781399	-1.333479	-1.908257
H	0.812065	2.661188	0.872394
H	0.113759	2.557566	-0.753899
H	2.401563	2.530201	-1.655788
H	3.072394	1.861214	-0.089384
H	-1.573866	1.758299	1.320873
H	-0.650810	-1.443521	-1.396809
H	-3.966977	1.177927	1.199307
H	-3.046568	-2.031787	-1.516303

H	-4.726706	-0.725570	-0.220701

8b-TSII

C	3.732075	-0.372979	0.378933
C	3.218104	0.927504	0.420127
C	1.886139	1.174331	0.094207
C	1.006901	0.133700	-0.292542
C	1.551896	-1.172420	-0.321238
C	2.885120	-1.419940	0.006035
C	-0.415083	0.386037	-0.597814
C	-1.486135	0.876266	1.020255
C	-2.086724	-0.274498	1.543716
C	-2.865334	-1.199824	0.654475
C	-1.886571	-1.808813	-0.382854
C	-1.224360	-0.733752	-1.276151
C	-2.089893	1.834633	-0.017045
C	-0.910168	1.784496	-1.003345
H	-3.334411	-2.002959	1.235297
H	-3.672092	-0.677533	0.120670
H	-2.425413	-2.512922	-1.032131
H	-1.125479	-2.390254	0.152926
H	-2.025777	-0.267303	-1.864445
H	-0.581167	-1.236605	-2.013508
H	-0.754930	1.363282	1.668283
H	-1.639347	-0.715507	2.434414
H	-1.166633	1.873509	-2.068464
H	-0.183263	2.568286	-0.777545
H	-2.329658	2.824280	0.391812
H	-3.006612	1.427148	-0.454381
H	1.526166	2.196565	0.149276
H	0.929072	-2.011983	-0.609492
H	3.859094	1.757588	0.708229
H	3.263518	-2.438844	-0.034555
H	4.771134	-0.565196	0.633051

8c

C	-0.709183	0.899969	0.720860
C	-1.936293	0.111047	0.990231
C	-2.372301	-1.000381	0.084852
C	-1.176868	-1.714848	-0.576010

C	-0.241859	-0.695322	-1.243681
C	0.378370	0.279484	-0.214103
C	0.629241	1.704381	-0.817822
C	-0.740404	2.149078	-0.245287
H	-2.990728	-1.719643	0.638586
H	-3.026745	-0.612526	-0.722326
H	-1.537570	-2.434201	-1.322326
H	-0.627471	-2.288436	0.183349
H	-0.820570	-0.114869	-1.976714
H	0.548062	-1.199956	-1.814687
H	-0.242033	1.203846	1.665107
H	-2.593409	0.424102	1.799276
H	0.769520	1.757942	-1.903521
H	1.463767	2.220613	-0.329303
H	-0.789133	3.132439	0.232920
H	-1.544584	2.077609	-0.984688
C	1.585949	-0.335350	0.482978
C	2.785609	-0.702677	-0.382433
H	2.854999	-0.090900	-1.287907
H	3.700866	-0.606418	0.207869
H	2.698682	-1.751959	-0.693957
O	1.615347	-0.521240	1.688851

8c-TSI

C	0.352334	0.296807	-0.140572
C	-0.698508	0.680136	0.911933
C	-1.901315	0.015422	1.042755
C	-2.397707	-0.983267	0.033917
C	-1.238977	-1.613537	-0.756823
C	-0.294483	-0.525281	-1.285698
C	-0.609024	2.405142	-0.279911
C	0.705721	1.738186	-0.625027
C	1.559384	-0.432884	0.458401
O	1.610287	-0.737213	1.638828
C	2.728133	-0.750083	-0.466755
H	-2.983426	-1.762733	0.539924
H	-3.098843	-0.500387	-0.671763
H	-1.628557	-2.208434	-1.592799
H	-0.686549	-2.302475	-0.103094
H	-0.868213	0.157497	-1.927971
H	0.485661	-0.957286	-1.924671
H	-0.304908	1.186353	1.790444

H	-2.557858	0.272559	1.872572
H	0.997742	1.794313	-1.682685
H	1.522283	2.163946	-0.029088
H	-0.623805	3.301282	0.335744
H	-1.427141	2.327731	-0.991785
H	2.816402	-0.043390	-1.298371
H	3.653853	-0.763893	0.114764
H	2.587714	-1.751240	-0.895169

8c-TSII

C	-0.492620	0.098519	0.506140
C	0.490776	1.046488	-0.938453
C	1.533930	0.217813	-1.372992
C	2.476833	-0.416954	-0.397847
C	1.661404	-1.414051	0.469877
C	0.550859	-0.713631	1.280055
C	0.544681	2.096382	0.183938
C	-0.652842	1.549524	0.979932
C	-1.600390	-0.674847	-0.090050
O	-1.491719	-1.892963	-0.262758
C	-2.874501	0.037568	-0.528655
H	3.280386	-0.949515	-0.919612
H	2.952801	0.325170	0.258936
H	2.336101	-1.925755	1.169520
H	1.214681	-2.179945	-0.173180
H	1.027690	-0.053414	2.017408
H	0.015069	-1.485300	1.849565
H	-0.262589	1.280225	-1.693279
H	1.407835	-0.285709	-2.330952
H	-0.605353	1.675308	2.069725
H	-1.589798	1.993983	0.631569
H	0.454956	3.126926	-0.181025
H	1.476477	2.022368	0.752626
H	-2.670835	0.891058	-1.186680
H	-3.510600	-0.677540	-1.055045
H	-3.421849	0.424976	0.340819

8d

C	1.047278	-0.057546	-0.744093
C	1.708993	1.245184	-0.979623

C	2.998797	1.599332	-0.302012
C	3.876850	0.362402	-0.027066
C	3.072069	-0.719791	0.707706
C	1.896140	-1.223000	-0.144725
C	0.652223	-1.669052	0.668749
C	0.031421	-0.253387	0.479275
H	3.549355	2.337701	-0.901459
H	2.801518	2.101817	0.666771
H	4.754821	0.653553	0.564045
H	4.252277	-0.039023	-0.979681
H	2.698486	-0.296769	1.652868
H	3.715218	-1.566085	0.984490
H	0.521962	-0.393200	-1.648677
H	1.173485	2.016094	-1.531584
H	0.815374	-1.997976	1.702173
H	0.073953	-2.439617	0.147621
H	0.344269	0.399475	1.301187
H	2.264602	-1.942178	-0.887285
C	-1.444242	-0.072967	0.251000
C	-2.157884	0.907216	0.959554
C	-2.150491	-0.851999	-0.682189
C	-3.525441	1.104914	0.749451
H	-1.632954	1.522549	1.687827
C	-3.516519	-0.659220	-0.896809
H	-1.629887	-1.620298	-1.249763
C	-4.211586	0.321136	-0.181142
H	-4.052913	1.870192	1.313982
H	-4.039758	-1.276079	-1.623689
H	-5.275448	0.470512	-0.347294

8d-TSI

C	-1.177289	0.019326	0.894091
C	-1.787736	1.277571	0.969185
C	-3.034450	1.609440	0.196813
C	-3.887433	0.356889	-0.077333
C	-3.025677	-0.762168	-0.679170
C	-1.893130	-1.192610	0.271689
C	-0.649488	-1.733096	-0.465162
C	0.061871	-0.387220	-0.589372
H	-3.620519	2.362507	0.741454
H	-2.775583	2.084233	-0.768766
H	-4.716472	0.604937	-0.752762

H	-4.335764	0.010821	0.865090
H	-2.598616	-0.402696	-1.627275
H	-3.640136	-1.636559	-0.931708
H	-0.474987	-0.225025	1.692812
H	-1.294708	2.075524	1.522482
H	-0.842215	-2.241387	-1.420349
H	-0.091501	-2.426812	0.171925
H	-0.336139	0.241162	-1.385736
H	-2.301502	-1.873144	1.032863
C	1.481288	-0.154147	-0.333987
C	2.086668	1.034044	-0.807396
C	2.288301	-1.037675	0.418088
C	3.423907	1.322802	-0.547581
H	1.488747	1.732266	-1.389925
C	3.628662	-0.749096	0.675103
H	1.867614	-1.963179	0.800893
C	4.206747	0.431457	0.196543
H	3.860284	2.242968	-0.929164
H	4.226418	-1.451577	1.251354
H	5.251633	0.652850	0.397747

8d-TSII

C	0.913877	0.004869	0.999029
C	1.787252	-1.022372	1.309221
C	2.704490	-1.621362	0.278751
C	3.741321	-0.547848	-0.144058
C	3.093606	0.672840	-0.843025
C	2.040750	1.435190	-0.058607
C	0.661249	1.592936	-0.675613
C	0.108613	0.197757	-0.304148
H	3.226825	-2.496244	0.684697
H	2.159711	-1.963593	-0.612857
H	4.479586	-0.991135	-0.826480
H	4.292197	-0.215082	0.747021
H	2.655384	0.324858	-1.790129
H	3.902126	1.366141	-1.126460
H	0.485607	0.548387	1.843605
H	2.114847	-1.101347	2.346155
H	0.648689	1.814539	-1.753616
H	0.094661	2.382104	-0.168348
H	0.462352	-0.527631	-1.044791
H	2.406212	2.207800	0.617921

C	-1.394086	0.034130	-0.174625
C	-2.066232	-0.963529	-0.895928
C	-2.154117	0.866010	0.663852
C	-3.450173	-1.128822	-0.787593
H	-1.497349	-1.621482	-1.550086
C	-3.536496	0.705406	0.778182
H	-1.664866	1.651059	1.236334
C	-4.191444	-0.293811	0.051539
H	-3.946823	-1.910003	-1.358157
H	-4.103011	1.361914	1.434399
H	-5.267802	-0.418650	0.138924

8e

C	-3.464452	0.607402	0.592384
C	-3.034558	0.832860	-0.719971
C	-1.867625	0.229214	-1.188038
C	-1.091615	-0.608605	-0.364755
C	-1.541104	-0.828138	0.944917
C	-2.713919	-0.228814	1.419630
C	0.156143	-1.232962	-0.951184
C	1.089234	-2.109028	-0.064521
C	2.150909	-0.977605	-0.016376
C	1.429193	-0.264608	-1.200796
C	1.334673	1.212445	-1.170627
C	1.589420	1.999186	0.078700
C	2.594273	1.300460	1.015944
C	2.159849	-0.148498	1.278058
H	1.937558	3.009804	-0.176786
H	0.643083	2.145030	0.635611
H	2.667430	1.853468	1.961314
H	3.594846	1.313766	0.559453
H	1.154707	-0.130767	1.721432
H	2.816805	-0.628644	2.016319
H	1.861468	-0.587320	-2.158283
H	0.958513	1.733851	-2.049354
H	0.702450	-2.449442	0.901602
H	1.437190	-2.992271	-0.611155
H	-0.133936	-1.729262	-1.884786
H	3.176688	-1.290346	-0.251250
H	-1.550701	0.404447	-2.214209
H	-0.982894	-1.478947	1.610730
H	-3.611719	1.475767	-1.380508

H	-3.038851	-0.422138	2.439338
H	-4.375169	1.073148	0.960349

8e-TSI

C	-3.510587	-0.851548	-0.406993
C	-3.220341	-0.474329	0.910247
C	-2.090307	0.289784	1.188533
C	-1.202378	0.698980	0.166338
C	-1.515867	0.310883	-1.153435
C	-2.653461	-0.448376	-1.434690
C	-0.018590	1.485472	0.534990
C	0.995000	2.042784	-0.473269
C	2.118289	1.009857	-0.218574
C	1.593274	0.522213	1.144028
C	1.572854	-0.838916	1.482822
C	1.801337	-1.922575	0.467804
C	2.708911	-1.433970	-0.676962
C	2.164853	-0.123619	-1.261874
H	2.237028	-2.804423	0.957296
H	0.839630	-2.263576	0.042845
H	2.774181	-2.199650	-1.460974
H	3.727885	-1.280191	-0.293411
H	1.154067	-0.318061	-1.642494
H	2.764195	0.201887	-2.122968
H	1.784610	1.204538	1.973897
H	1.309833	-1.128750	2.499104
H	0.647632	2.090601	-1.512351
H	1.297010	3.057560	-0.188385
H	-0.210680	2.123380	1.397371
H	3.120484	1.455571	-0.132880
H	-1.878483	0.581054	2.215588
H	-0.877552	0.620624	-1.975036
H	-3.881040	-0.773818	1.720555
H	-2.872272	-0.722224	-2.464285
H	-4.394448	-1.444375	-0.627658

8e-TSII

C	-3.462018	0.398893	0.598636
C	-2.992475	0.871566	-0.632315
C	-1.781832	0.408318	-1.145594

C	-0.999992	-0.530451	-0.446934
C	-1.490719	-1.003060	0.777215
C	-2.706836	-0.542524	1.297540
C	0.285144	-1.026942	-1.101881
C	1.207468	-2.002320	-0.327627
C	2.308490	-1.044857	0.099214
C	1.363743	0.043755	-1.447297
C	1.488738	1.370180	-1.077814
C	1.186265	1.876418	0.304535
C	2.243184	1.285551	1.273151
C	2.147465	-0.255226	1.384849
H	1.233977	2.972190	0.334203
H	0.186112	1.585045	0.645279
H	2.110966	1.716790	2.274910
H	3.247650	1.574570	0.932605
H	1.176368	-0.494807	1.837641
H	2.909314	-0.589766	2.108280
H	1.901553	-0.232594	-2.356528
H	2.216671	1.956187	-1.641042
H	0.733036	-2.550063	0.497857
H	1.601430	-2.757608	-1.017424
H	-0.032441	-1.478886	-2.053063
H	3.332141	-1.272831	-0.198798
H	-1.426173	0.786884	-2.100994
H	-0.931999	-1.741081	1.343738
H	-3.572192	1.600255	-1.194057
H	-3.060074	-0.926767	2.251620
H	-4.406093	0.756685	1.001703

8f

C	0.171593	0.138030	-0.740448
C	0.939015	1.397371	-0.668139
C	2.224133	1.485469	0.098162
C	2.999931	0.152380	0.089853
C	2.094177	-1.001733	0.541922
C	0.904568	-1.201210	-0.411257
C	-0.387194	-1.717013	0.274125
C	-0.893397	-0.263026	0.412039
H	2.845457	2.298295	-0.301416
H	2.027285	1.760629	1.153906
H	3.876823	0.229260	0.745365
H	3.375586	-0.045461	-0.924425

H	1.730074	-0.783236	1.557755
H	2.662435	-1.938489	0.617041
H	-0.364478	0.054351	-1.694258
H	0.516952	2.303199	-1.100564
H	-0.266122	-2.284030	1.204177
H	-1.030718	-2.279241	-0.408702
H	-0.599613	0.202429	1.358547
H	1.232782	-1.757632	-1.298235
C	-2.330495	0.060075	0.082452
C	-2.872973	1.376692	0.609176
H	-2.980799	1.322255	1.701083
H	-2.173261	2.196655	0.400738
H	-3.846370	1.592758	0.162498
O	-3.012773	-0.679244	-0.612602

8f-TSI

C	0.309616	0.183233	-0.864189
C	1.026406	1.377612	-0.720509
C	2.285601	1.465671	0.093888
C	3.013549	0.110667	0.169551
C	2.041317	-1.001722	0.585918
C	0.888585	-1.173107	-0.421110
C	-0.413868	-1.689213	0.224043
C	-1.003914	-0.318395	0.528009
H	2.944153	2.237970	-0.326324
H	2.052428	1.808242	1.119323
H	3.849557	0.173156	0.877612
H	3.445548	-0.123678	-0.813802
H	1.634017	-0.757460	1.578617
H	2.567771	-1.958463	0.698605
H	-0.391092	0.128596	-1.697788
H	0.624457	2.293254	-1.152441
H	-0.280791	-2.336691	1.100284
H	-1.051755	-2.205384	-0.499619
H	-0.643180	0.179644	1.427562
H	1.239071	-1.765910	-1.277906
C	-2.357898	0.059814	0.101564
C	-2.927937	1.348991	0.674108
H	-3.180849	1.211684	1.734107
H	-2.193781	2.163348	0.621176
H	-3.832061	1.630699	0.129077
O	-2.994029	-0.607539	-0.718265

8f-TSII

C	-0.017762	0.348374	0.914065
C	-0.947160	1.370054	0.873970
C	-1.904680	1.523884	-0.275831
C	-2.875472	0.313905	-0.270995
C	-2.162262	-1.036225	-0.531006
C	-1.055283	-1.431539	0.429632
C	0.327460	-1.706208	-0.137905
C	0.783858	-0.247513	-0.268501
H	-2.477137	2.454785	-0.184441
H	-1.387736	1.564131	-1.245476
H	-3.646839	0.453994	-1.040502
H	-3.395619	0.278891	0.696544
H	-1.758949	-1.013007	-1.554318
H	-2.930560	-1.826180	-0.532325
H	0.447650	0.139901	1.879480
H	-1.274504	1.780222	1.829578
H	0.340881	-2.276190	-1.078575
H	0.964761	-2.230151	0.581043
H	0.424341	0.198801	-1.203799
H	-1.362259	-1.941502	1.342660
C	2.280846	0.034467	-0.146661
C	2.740929	1.429979	-0.523834
H	2.689586	1.547323	-1.615176
H	2.081486	2.190001	-0.088191
H	3.771488	1.589565	-0.197703
O	3.061321	-0.813206	0.254200

8g

C	-0.246637	0.150107	-1.231021
C	-0.656927	-1.259182	-1.027647
C	-1.569655	-1.672578	0.088042
C	-2.514852	-0.535939	0.524618
C	-1.715079	0.739834	0.823172
C	-1.001859	1.260953	-0.434248
C	0.344943	1.991265	-0.174037
C	1.144149	0.754256	-0.653495
H	-2.143189	-2.561541	-0.210180
H	-0.979986	-1.986053	0.971233

H	-3.080645	-0.847706	1.411789
H	-3.249739	-0.342824	-0.270986
H	-0.975462	0.518673	1.603430
H	-2.369096	1.526721	1.222572
H	-0.236504	0.381824	-2.304832
H	-0.235098	-2.027768	-1.674180
H	0.531327	2.281809	0.864301
H	0.502168	2.858971	-0.823186
H	1.867377	0.934575	-1.457308
H	-1.716637	1.816792	-1.054543
C	1.810755	-0.088755	0.413569
C	2.789092	-1.141273	-0.078115
H	2.367188	-1.708434	-0.916390
H	3.699589	-0.649533	-0.447361
H	3.055829	-1.818889	0.736339
O	1.582411	0.053907	1.605535

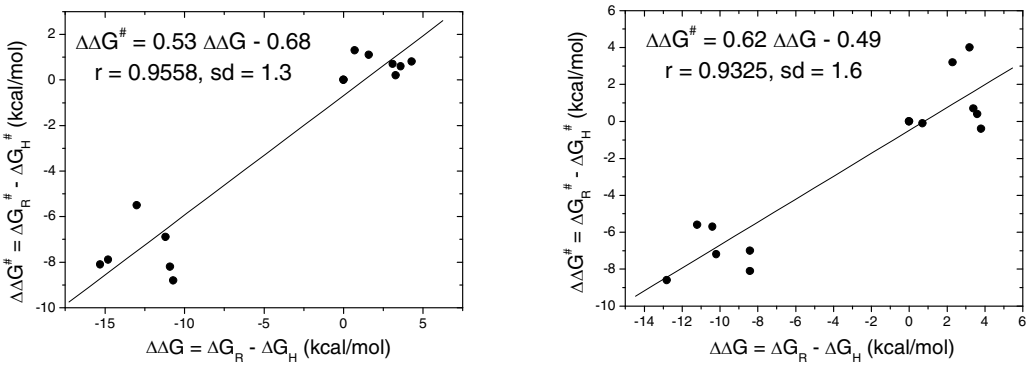
8g-TSI

C	-0.440218	0.131707	-1.307615
C	-0.860183	-1.195751	-1.131538
C	-1.647949	-1.634797	0.069061
C	-2.492778	-0.480141	0.640519
C	-1.615674	0.755898	0.880943
C	-0.966755	1.274445	-0.417550
C	0.401520	1.961580	-0.189858
C	1.285462	0.784737	-0.602210
H	-2.283362	-2.489604	-0.199941
H	-0.967033	-2.004758	0.856209
H	-2.966846	-0.794562	1.578835
H	-3.303851	-0.241827	-0.063206
H	-0.828444	0.494659	1.597791
H	-2.202292	1.565984	1.334409
H	-0.211559	0.416548	-2.335658
H	-0.559838	-1.947622	-1.860601
H	0.572227	2.287674	0.841607
H	0.555875	2.817767	-0.856137
H	1.898830	0.897507	-1.496089
H	-1.690953	1.896092	-0.963950
C	1.866847	-0.115702	0.405324
C	2.841531	-1.168852	-0.100960
H	2.372246	-1.782688	-0.881338
H	3.725478	-0.697277	-0.549577

H	3.155875	-1.810395	0.725544
O	1.562854	-0.060780	1.599426

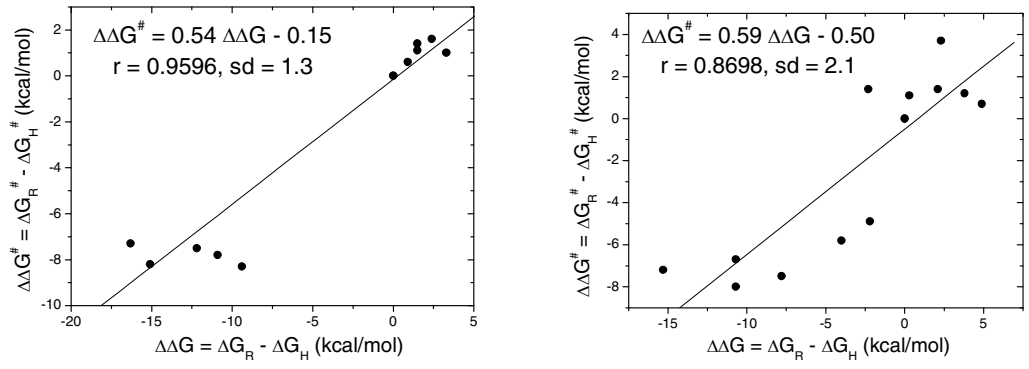
8g-TSII

C	0.136118	-0.026975	1.467096
C	0.715047	-1.252865	1.195638
C	1.057713	-1.711547	-0.195040
C	2.193662	-0.804342	-0.736184
C	1.748671	0.667865	-0.910877
C	1.232284	1.379562	0.325405
C	-0.161446	1.989395	0.287818
C	-0.980645	0.759268	0.721428
H	1.393519	-2.755752	-0.184306
H	0.206027	-1.658598	-0.884866
H	2.535016	-1.181859	-1.709369
H	3.053110	-0.861631	-0.053220
H	0.973458	0.696344	-1.686864
H	2.606693	1.231711	-1.312036
H	0.219444	0.308716	2.502026
H	1.325354	-1.680109	1.992061
H	-0.456002	2.380583	-0.693913
H	-0.262160	2.795615	1.023136
H	-1.767646	1.004561	1.452403
H	1.981272	1.837942	0.971542
C	-1.713135	0.016894	-0.398853
C	-2.575866	-1.159073	0.023039
H	-2.042123	-1.813339	0.720594
H	-3.466018	-0.782872	0.545796
H	-2.897870	-1.720093	-0.857581
O	-1.664561	0.381211	-1.562778



(a) (b)

SFigure 1. Correlation between the relative activation and reaction free energies for (a) bicyclo[3.2.0]heptan-1-ylmethyl and (b) bicyclo[2.2.0]heptan-2-yl radicals.



(a) (b)

SFigure 2. Correlation between the relative activation and reaction free energies for (a) bicyclo[4.2.0]octan-1-ylmethanyl and (b) bicyclo[2.2.0]octan-2-yl radicals.